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PATENT APPLICATION TRANSHITTAL LETTER



# SN 08/247,884

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### MODEL FOR TESTING IMMUNOGENICITY OF PEPTIDES

#### Government Interest

The invention described herein may be manufactured, licensed and used by or for governmental purposes without the payment of any royalties to us thereon.

### Cross Reference

This application is a continuation in part of U.S. Patent Application Serial No. 08/789,734 filed January 27, 1998 which in turn is a continuation in part of U.S. Patent Application Serial No. 08/590,973 filed January 24, 1996 which in turn is a continuation in part of U.S. Patent Application Serial No. 08/247,884 filed May 23, 1994 which in turn is a continuation-in-part of U.S. Patent Application Serial No. 08/064,559, filed May 21, 1993 Mand the present application incorporates U.S. Patent Application Serial Nos. 08/064,559, 08/789,734, 08/590,973 and 08/247,884 in their entirety by reference.

#### Field of the Invention

This invention relates to a means of predicting potential of a peptide for eliciting immune response.

### Background of the Invention:

Among the numerous steps required for an immunological response to occur is the presentation of the antigen by macrophages to the B-cell or T-cell. This presentation is mediated by the Class I and Class II major histocompatibility complex (MHC) molecules on the surface of the cell. The MHC molecules hold antigens in the form of the peptide fragments and together with the receptor molecule on the T-cells,

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form a macromolecular complex that induces a response in the T-cell. Therefore, a necessary step in an immune response is the binding of the antigen to the MHC.

Recent single crystal X-ray structures of human and murine Class I MHC's have been reported. Analysis of these crystal structures have shown that antigenic peptides lie in the so-called binding cleft for presentation to the T-cell. This cleft is formed by  $\alpha_1$ and  $\alpha_2$  domains and by 6-strands from each domain forming the floor. Furthermore, the sequence polymorphism among Class I molecules can result in alterations of the surface of the cleft forming different pockets. Peptide side chains may insert into these pockets. Thus, different pockets may interact with different side chains. This implies the mechanism for the peptide specificity of class I MHC's. bound to the Class I MHC's in the crystal structures were found to have both the amino and carboxy termini tightly held by the MHC. There were few interactions near the middle of the cleft. Hence the bound peptide is allowed to bend slightly in the center. observed binding mode helped to explain the apparent partial specificity of peptide sequence and the allowed variation in peptide length found among peptides isolated from Class I MHC's.

The precise mode of binding of peptides to Class
II MHC molecules is less clear. While a single crystal
X-ray diffraction structure for the HLA-DR1 MHC has
been shown, the coordinates have remained unavailable.
However, currently available theoretical and
experimental results help form a hypothesis that the
binding of a peptide to Class II MHC is similar to that

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observed with Class I. First, it is noted that the Class II binding cleft is structurally similar to that of Class I. This was concluded based upon a sequence analysis of 26 Class I and 54 Class II amino acid sequences.

Unlike with Class I molecules, self-peptides isolated from murine I-A<sup>b</sup> and I-E<sup>b</sup>, from murine I-A<sup>d</sup> and from human HLA-DR1 molecules were found to be varied in size (13 to 25 residues long). The peptides isolated from the murine I-A<sup>b</sup> and I-E<sup>b</sup> molecules had heterogenous carboxy termini while those from I-A<sup>d</sup> and HLA-DR1 had ragged termini at both ends. The varying lengths indicate that the amino and carboxy termini of the peptides were not critical for the binding. One or both termini may protrude from the binding site and be available for further processing. The residues critical for binding were proposed to be at the ends of the peptide as opposed to the center.

### Summary of the Invention:

It is the purpose of this invention to provide a method for preliminary screening of peptides for ability to elicit an immune response. Structural homology techniques were used to model a receptor (the Class II MHC is exemplified). This model makes it possible to preliminarily screen peptides for antigenic properties. By modifying the peptide to "fit" into the receptor it is possible to identify methods of rendering non-immunogenic peptides immunogenic.

The preliminary screening of peptides for immunogenicity comprises the steps of (1) creating a molecular model of a receptor followed by minimizing the model created, 2) modeling a peptide to be tested

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and minimizing the model of the peptide, then testing the fit of the model of the peptide into the model of the receptor to produce a composite minimized receptor/minimized peptide model. Upon finding an acceptable fit, the peptide may then be screened by a binding assay for actual binding to Class II MHC as a further test for immunogenicity.

It has been found that when the model of the peptide can not be fitted into the model of the receptor, the peptide will lack immunogenicity. While he all peptide models which can be made to "fit" into the model of the receptor will be effective as immunogens, the screening methods of the invention may make it possible to avoid undue biological testing of inappropriate peptides. By using the model, it is also possible to alter peptides to accommodate the receptor. Hence, the invention has both predictive and drug design applications.

### Brief Description of the Figures:

Fig. 1 shows the HLA-aw68  $\alpha_1$  and  $\alpha_2$  domains with DR1  $\alpha_1$  and  $\beta_1$  domains aw68  $\alpha_1$ , and  $\alpha_2$  domains are represented by SEQ ID NO:13, DR1  $\alpha$ , and  $\beta_2$  domains are represented by SEQ ID NO:14 and SEQ ID NO:15 respectively,

Figs. 2-30 are a printout of the minimized goordinates of the receptor,

Figs. 31 and 32 shows the effects of various peptides inhibiting the binding of labeled hemagglutinin in a competitive binding assay.

#### Detailed Description of the Invention:

In order to understand and better predict peptide interaction with Class II MHC's and as an aid for

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synthetic peptide vaccine design, a structural homology model of HLA-DR1 molecule was made using the Class 1 HLA-aw68 as a reference molecule. For purposes of this analysis, numerous conserved residues were aligned leading to a proposed three-dimensional model for the Class II structure very similar to that of Class I. This model retained the overall conformation of a Class I MHC and agreed with a considerable amount of the published data. Furthermore, peptides shown to bind to DR1 were docked in the binding cleft of the model and analyzed. The results agree with the experimental binding data presented here. Hence, it is shown that the structural homology model reported here is useful for screening Class II MHC functionality.

It had been hypothesized that few peptide residues may be required for binding to DR1. By substituting residues into the influenza hemagglutinin 307-319 T-cell epitope (HA) it had been determined that a single tyrosine at 308 was required for binding. A synthetic peptide with the tyrosine at position 308 and a lysine at 315 was found to bind DR1 as well as the native peptide. Hence, it was concluded that few peptide residues determine the high affinity binding to DR1.

The peptides produced according to the present invention may be used alone or chemically bound to another peptide and/or carrier in order to elicit an immune response. An immune response is elicited by administering a peptide to an animal in an effective dose and by an effective route of administration. Typically the peptide will be administered with an immunologically acceptable carrier. The routes of administration, dosages, times between multiple administrations will be based on the particular peptide and are standard operations of those skilled in the art.

Of particular interest are peptides from pathogenic microorganisms and neoplasms. In such an example, a vaccine may be formed with the peptide and any known immunological carrier and may be administered prophylactically or therapeutically. The immune response may be elicited for a number of reasons other than for prophylaxis or therapy such as increasing antibody production form the harvesting of antibodies, or increasing specific B-cell or T-cell concentration for the production of hybridomas or cellular therapy.

The choice of host animals is limited only to those capable of an immune response. Preferred hosts are mammals, more preferred are humans.

The vaccine may contain plural peptides with each peptide corresponding to the same or different antigens. The peptides may be used unbound or they may be chemically bound to another peptide or an unrelated protein or other molecule. A preferred vaccine preparation contains a plurality of peptides chemically bound to a larger more immunogenic peptide.

The peptide or plurality of peptides may be adsorbed, bound or encapsulated in a biodegradable microsphere, microcapsule, larger carrier or a combination of these. The carrier may have a slow or controlled release property thereby releasing the peptide under appropriate conditions and times for enhanced immunization. This is particularly important when administering the peptide orally where stomach acid can degrade the peptide.

When the peptide is combined (i.e. encapsulated within) with a biodegradable lactide and/or glycolide polymers, they can be formulated into immunostimulating composition comprising encapsulating- microspheres, which may contain a pharmaceutically-acceptable adjuvant, wherein said microspheres having a diameter

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between 1 nanogram (ng) to 10 microns (um) are comprised of (a) a biodegradable-biocompatible poly (DL-lactide-co-glycolide) as the bulk matrix, wherein the relative ratio between the amount of lactide and glycolide components are within the range of 40:60 to 0:100 and (b) an immunogenic substance comprising Colony Factor Antigen (CFA/II), hepatitis B surface antigen (HBsAg), or a physiologically similar antigen that serves to elicit the production of antibodies in animal subjects. Compositions wherein the immunogenic substance is a peptide within the range of 0.1 to 1.5% based on the volume of the bulk matrix of lactide and glycolide component having a relative to 58:42 should be especially useful.

Another embodiment of the present invention is to modify the amino acid sequence of a peptide to enhance its immunogenicity. This is done by modifying the natural peptide sequence to bind to the Class II MHC receptor DR12 with superior binding affinity for a Class II MHC receptor DR1 than the natural peptide sequence. This modified peptide is considered a synthetic peptide. Alternatively, the sequence may be modified to have a greater inhibition of HA (306-318) binding to a Class II MHC receptor DR1.

Many amino acid changes are acceptable in the formation of a synthetic peptide. The changes may be for similar types of amino acids such as leucine for isoleucine or they may be for diverse types such as tyrosine for lysine.

### Materials and Methods:

The structural homology model for the DR1 Class II MHC was constructed using the QUANTA molecular modeling package (vision 3.2, Molecular Simulations, Inc., Burlington, MA) with the CHARMM and Protein Design modules. After alignment of the sequences as described

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below, gaps and loops were energy minimized using 100 steps of steepest descents minimization followed by 100 steps of adopted basis set Newton-Rapheson (ABNR) minimization. Large gaps were closed using a fragment database from a selected set of high-resolution crystal structures. The resulting structure we minimized in vacuo using 1000 steps of steepest descents followed by an additional 1000 steps of ABNR minimization. distance related electrostatic function was used in all calculations with a dielectric constant of 1.0. Nonbound parameter lists were updated every 20 steps with a cutoff distance of 15.0A. Non-bonded calculations were performed using a shifted potential function between 11.0A and 14.0A. An extended atom set was used with only polar hydrogen atoms specifically placed. There were no explicit hydrogen bond energy calculations performed.

All peptides were initially modeled using QUANTA in an extended chain conformation and subjected to 500 steps of ABNR minimization. The resulting structures remained essentially in extended chain conformations. Individual peptides were manually docked in several different orientations into the binding cleft region of the minimized DR1 structure. The resulting bimolecular complex was subjected to 5000 steps of steepest descents minimization with non-bonded interactions updated every five steps. After minimization, bound peptides remained essentially in extended chain conformations. The lowest energy complexes for each peptide were selected for further analysis.

The selected peptide and DR1 complexes and the minimized DR1 model were subjected to the following molecular dynamics regimen: 300 steps of heating to 300°K, 600 steps of equilibration at 300°K, and 1100 steps of production dynamics. During this simulation,

the DR1 C $\alpha$  atoms were constrained in their starting positions. All non-bonded interaction parameters were as stated for the minimization procedure. The lowest energy structure during the course of the production dynamics was selected and subjected to the 5000 step minimization procedure described previously with the C $\alpha$  restraints removed. The resulting structures were used for the binding energy calculations and for hydrogen bonding analysis.

Hydrogen bonds were determined using the QUANTA default parameters. Maximum allowed distances were 2.5Å between a hydrogen and the acceptor atom and 3.3Å between the donor and acceptor atoms. The minimum angle allowed between any set of atoms forming a hydrogen bond was 90°.

# Competitive Inhibition Binding Assay:

HA peptide (the influenza hemagglutinin 307-319 T-cell epitope) was labeled with <sup>125</sup>I. The labeled HA peptides were then allowed to interact with purified DR1 molecules during incubation to allow formation of peptide/DR1 complexes. After incubation, the peptide/DR1 composition was exposed to a native gel for chromatographic separation or passed through a spun column to separate labeled peptide/DR1 complex and free labelled peptide. When unlabeled peptides were added before incubation of labeled HA peptides and DR1, and if the unlabelled peptides had capacity for binding to DR1 simultaneous with <sup>125</sup>I-HA, there was a resultant decrease in radioactive signal associated with the DR1. The extent of this decrease directly related to the binding capacity of the unlabeled unknown peptide.

# Structural Homology Model for the DR1 Molecule:

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The structural homology model was created, the reference molecule being the crystal structure of HLA-aw68. The HLA-aw68 coordinates and subsequent sequence were obtained from the entry 2HLA in the Brookhaven Protein Data Bank released January 15, 1991, which is incorporated herein by reference. The sequence for the DR1 molecule was for the  $\alpha_1$  domain was reported by Klein and for the  $\beta_1$  domain, the study reported by Todd et al. (Nature 329, 599 (1987)).

The sequence alignment is based on Brown et al. (Nature 332, 845 (1988)). The complete alignment and numbering scheme for both are seen in Figure 1. Class II,  $eta_1$  and Class I  $lpha_2$  domains regions were conserved with some variations at the ends where the two MHC's have different loop regions. The fourth Bstrand in the  $\alpha_1$  domain of HLA-aw68 (residues 30-38) is disrupted in the DR1 model. Only three residues are in a  $\beta$ -sheet conformation, probably due to the inserted glycine at position 28 before the strand and the large deletion in the loop region immediately after the strand. The two alpha-helical regions are clearly maintained. Both helices have been observed to be discontinuous in the Class I molecules and are similar in the DR1 model. The  $\alpha_1$  domain helix is long and curves from residues  $49\alpha$  to  $76\alpha$  without significant It is essentially a single continuous disruption. helix. However, the  $\alpha_2$  helical region is broken into two separate helices as with the Class I molecules. A short helix (52-63) is separated from a longer helix (68-94) by a deformed region without secondary structure. This deformation is more pronounced in the DR1 model as opposed to the Class I molecules due to an insertion.

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# Influenza Hemagglutinin Peptide with DR1:

The amino acid residues 307-319 of influenza hemagglutinin (Pro-Lys- Tyr-Val-Lys-Gln-Asn-Thr-Leu-Lys-Leu-Ala-Thr, SEQ ID NO:1) make up a well-documented linear T-cell epitope which as been shown to be HLA-DR1 restricted. With the demonstration that the influenza hemagglutinin epitope (referred to as the HA peptide) binds DR1, it was chosen to be modeled into the binding cleft.

The peptide was initially inserted into the cleft so that Leu 11 HA was in the vicinity of the hydrophobic pocket. This allowed Asn 7 to be near the middle charged and polar groups of the cleft. The remaining residue of the motif (Lys 2) was near the vicinity of the remaining charged and polar residues at the end of the cleft. The only adjustment to the starting conformation was a slight rearrangement of the terminal peptide proline and Tyr 3 to alleviate obvious bad contacts.

After the energy minimization of the bimolecular complex, the total energy was reduced to 483 kcal/mol. This reduction in energy was accomplished by alleviation of several bad contacts and also be formation of several hydrogen bonds. The sticking feature of this mode is lack of hydrogen bonds in the carboxy terminal half of the peptide. Only one hydrogen bond is identified between the backbone carbonyl group of Leu 9 and the side chain of the  $\beta_1$  Asn 77. In contrast, the amino terminal half has eleven identified interactions. Four of these interaction involve the peptide backbone residues Tyr 3, Val 4, and Gln 6. The remainder involve the side chains of Lys 2, Tyr 3, Lys 5 and Gln 6. Interestingly, Lys 5 is involved in more interactions

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(three) than Lys 2 (only 2). No interactions were observed as anticipated with Asn 7. Instead it was the glutamine at position 6 donating a hydrogen bond to the  $\alpha_1$  Asn 62. No interactions were observed for the amino and carboxy termini.

## HA-YK Peptide with DR1:

The binding of the HA-YK peptide (Ala-Ala-Tyr-Ala-Ala-Ala-Ala-Ala-Lys-Ala-Ala, SEQ ID NO:2) to the DR1 model was tested. In aligning the peptide in the cleft, it was deemed logical to insert the tyrosine residue into the hydrophobic region of the binding The lysine would then be in position to interact with the hydrophilic groups in the other half of the cleft. The resulting peptide orientation is the opposite that used for the HA and the CS3 (defined below) peptides. With the peptide oriented as described, the final docking position for the peptide was unclear. The hydrophobic pocket is quite large, and, at least in this model, could accommodate the peptide tyrosine in a number of positions by sliding the peptide lengthwise through the cleft. However, repositioning the peptide also repositions the lysine. There were primarily two positions for the lysine: one with the lysine inside the cleft and the second with it outside. Of the two positions, the former was the lower in energy by 46 kcal/mol and had the greater number of interactions with the protein (11 vs. 7). Thus, the preferred orientation of the peptide appears to be with the lysine inside the binding cleft region.

## CS3 subunit Pilin Peptide with DR1:

The suspected T-cell epitope for CS3 pilus subunit 63-78 (Ser-Lys-Asn-Gly-Thr-Val-Thr-Trp-Ala-His-Glu-Thr-

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Asn-Asn-Ser-Ala, SEQ ID NO:3) was modeled with the DR1 molecule. The peptide was inserted with lysine inside the cleft in the hydrophilic region. This placed the Thr 5 in the center of the binding cleft and the tryptophane (residue 8) near the hydrophobic region. The resulting minimized model had ten interactions between the peptide and the protein, three interactions with the peptide backbone and five with the peptide side chains. The remaining two were with the amino terminal of the peptide. All of the interactions were in either the first three residues, His 10 or Glu 11 in the peptide. No interactions were observed in the center of the cleft or residues four through nine.

### CFA/1 with DR1:

A peptide identified as CFA/1 (colonization factor antigen) (Val-Gly-Lys-Asn-Ile-Thr-Val-Thr-Ala-Ser-Val-Asp-Pro, SEQ ID NO:4) was prepared and an attempt was made to "fit" the molecule into the cleft of the DR1. The lysine at position 3 prevented insertion of the peptide.

### Results:

The peptides chosen to dock in the DR1 model are shown in Table 1. The peptides were docked manually in several orientations into the DR1 model. The peptides were then tested in biological binding assays with the following results:

Table I

Peptide	Molecular Model predicted binding	Binding in the bioassay
HA (influenza hemagglutinin)	Yes	Yes
HA-YK (synthetic peptide)	Yes	Yes
CS3 Pilin subunit	Yes	Yes
CFA/1	No	No

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Quantitative measurement of the inhibition of CS3 63-78 and HA 306-318 as compared to controls is shown in Fig. 31.

The binding energy was calculated as the difference between the final DR1 and peptide complex and the sum of the energies for the minimized DR and peptide models individually. The data is shown in Table II.

Table II.

Peptide	Protein	Residues	Sequence	Binding Energy (kcal/mol)
НА	Influenza hemagglutinin	306-318	PKYVKQNTLKLAT, SEQ ID NO:1	-283
HA-YK	synthetic peptide		AAYAAAAAAKAA, SEQ ID NO:2	-216
CS3	CS3 pilin subunit	63-78	SKNGTVTWAHETNNSA, SEQ ID NO:3	-245

### $CS6\alpha$ and $CS6\beta$ with DR1

Colonization factor antigen IV (CFA/IV is an antigen on the surface of many entotoxigic *E. coli* one component of which is CS6. CS6 has two major subunits and a number of minor subunits. Several peptides from CS6 have been sequenced and assayed for potential inhibition of radiolabeled HA (306-318)/DR1 complex as a measure of immunogenicity. The sequences of the subunits are shown in Table III.

		/
Amino Acid Residues	Sequence	
63-75	DEYGLGRLVNTAD,	SEQ ID NO:5
80-92	IIYQIVDEKGKKK,	SEQ ID NO:6
111-123	LNYTSGEKKISPG	SEQ ID NO:7
3-15	WQYKSLDVNVNIE	SEQ ID NO:8
42-54	QLYTVEMTIPAGV	SEQ ID NO:9
112-124	TSYTFSAIYTGGE	SEQ ID NO:10
123-135	GEYPNSGYSSGTY	SEQ ID NO:11
133-145	GTYAGHLTVSFYS	SEQ ID NO:12
	63-75 80-92 111-123 3-15 42-54 112-124 123-135	63-75 DEYGLGRLVNTAD, 80-92 IIYQIVDEKGKKK, 111-123 LNYTSGEKKISPG 3-15 WQYKSLDVNVNIE 42-54 QLYTVEMTIPAGV 112-124 TSYTFSAIYTGGE 123-135 GEYPNSGYSSGTY

These peptides were assayed for inhibition of radioactivity labeled HA(306-318)/DR1. The results are demonstrated in Fig. 32.

The foregoing description of the specific embodiments reveal the general nature of the invention so that others can, by applying current knowledge, readily modify and/or adapt for various applications such specific embodiments without departing from the generic concept, and, therefore, such adaptations and modifications should and are intended to be comprehended within the meaning and range of equivalents of the disclosed embodiments. It is to be understood that the phraseology or terminology employed herein is for the purpose of description and not of limitation.

All references mentioned in this application are incorporated by reference.

- 1. A method of preliminarily screening peptides for immunogenicity comprising the steps of:
- 1) creating a molecular mode of receptor DR1 Class II MHC and minimizing the model of the DR1;
- 2) modeling a peptide to be tested and minimizing the model of the peptide; and
- 3) testing fit of model obtained in step 2 into the model obtained in step 1 to produce a composite receptor/peptide model.
- 2. A computerized model comprising a model of the DR1 molecule having fitted in a cleft therein a model of a peptide.
- 3. A method of claim 1 wherein, additionally, the receptor/peptide model is subjected to computer-simulated heating.
- 4. A method of claim 1 further comprising, assaying the peptide by competitive inhibition binding to a Class II MHC receptor DR1.
- 5. A minimized peptide capable of binding to a Class II MHC receptor DR1 and inhibiting the binding of HA (306-318).
- 6. A synthetic peptide, wherein the amino acid sequence of the
  minimized peptide according to claim 5 has been modified to have a
  superior binding affinity for a Class II MHC receptor DR1 to form at
  least a portion of the synthetic peptide.

- 7. A synthetic peptide, wherein the to acid sequence of the minimized peptide according to claim 5, has been modified to have greater inhibition of HA (306-318) binding to a Class II MHC receptor DR1 to form at least a portion of the synthetic peptide.
- 8. A synthetic peptide according to claim 6, wherein an amino acid has been modified from a charged amino acid to an uncharged amino acid.
- 9. A synthetic peptide according to claim 7, wherein an amino acid has been modified from a charged amino acid to an uncharged amino acid.
  - 10. A synthetic peptide according to claim 8, wherein said uncharged amino acid is alanine.
  - 11. A synthetic peptide according to claim 9, wherein said uncharged amino acid is alanine.
  - 12. A minimized peptide according to claim 5, wherein the sequence is selected from the group consisting of PKYVKQNTLKLAT, AAYAAAAAAKAA and SKNGTVTWAHETWNSA. SEQ ID NO:1, SEQ ID NO:2 and SEQ ID NO: 3 respectively
- 13. A minimized peptide according to claim 5, wherein the sequence is contained in a CFA.

14. A minimized peptide according to claim 13, wherein the sequence is selected from the group consisting of DEYGLGRLVNTAD, /IYQIVDEKGKKK, LNYTSGEKKISPG, WQYKSLDVNVNIE, QLYTVEMTIPAGV, TSYTFSAIYTGGE, GEYPNSGYSSGTY and GTYACHLTVSFYS, SEQ ID NO:5, SEQ ID NO:6, SEQ ID NO:7, SEQ ID NO:8, SEQ ID NO:9, SEQ ID NO:10, SEQ ID NO:11 and SEQ ID NO:12 respectively.

15. A vaccine comprising:

a minimzed peptide according to claim 5; and an immunologically acceptable carrier.

16. A vaccine comprising:

a synthetic peptide according to claim 6; and
an immunologically acceptable carrier.

17. A vaccine comprising:

a synthetic peptide according to claim 7; and
an immunologically acceptable carrier.

- 18. A method of eliciting an immune response in an animal comprising administering said animal with the vaccine according to claim 15.
- 19. A method of eliciting an immune response in an animal comprising administering said animal with the vaccine according to claim 16.
- 20. A method of eliciting an immune response in an animal comprising administering said animal with the vaccine according to claim 17.

# Abstract of the Invention

Assay methods for determining whether a peptide is likely to be immunogenic are based on a computer modeling of binding to a Class II MHC DR1 receptor. This is confirmed by competitive inhibition binding assays. The peptides are useful for eliciting an immune response for vaccination or the production of antibodies or T-cells.

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D 38 SDAKSQRUEP A8 RAPWIEQECP D 38 SDAKSQRUEP A8 RAPWIEQECP D 38 SDAKSQRUEP A8 RAPWIEQECP	GSH 94 TIQHAYGCDV 104 GSDGRFLRGY GSH 94 TIQHAYGCDV 104 GSDGRFLRGY A A A A A A A A A A A A A A A A A A A	(((((( * ballx )))))))))))))))))))))))))))))))))))		· 34	<b>-</b>
CSHSHRYF 9 YISVSRPCRC 19 EPRPIAVCYV 29 D DIQFYRPD 38 SDAASQREE AB RAPWIEQECP CSHSHRYF 9 YISVSRPCRC 19 EPRPIAVCYV 29 D DIQFYRPD 38 SDAASQREE AB RAPWIEQECP IXEEDVIIQA 11 EFYLR PDQ 19 SG EFHFDP 27 DGDEIFHYDH 37 AXX 40 EIVWRLEEPG	((((((( " helix ))))))))))))))))))))))))))))))))))))	114 RQDAYDGKDY 124 IALKEDLRSW 134 IAADHAA QI 143 IKUKWEAA H 152 VAEQHRAYLE 162 GTCVEWILRRY  28 ERCIYHQEES 38 WIFDSDVGEY 48 RAVTELGRPD 58 AEY WRSQKD 67 LLEQRRRAVD 77 IYCRHHYGVG			Conserved residues
1 GSUSPRYF 9 YIS' 1 IKEEUVIIQA 11 EFY	((((((( " helix )))))))))))))))))))))))))))))))))))	114 RQDAYDGKDY 124 + + + + + + + + + + + + + + + + + + +	172 LENGKETLQR	87 ESFTVQRRVII	
av68 DR1 E,	DR1 8, 2068 DR1 4,	DR1 8, av68 DR1 4, DR1 6,	3002	DR1 ", DR1 B,	

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\* MINIMIZED COORDINATES FROM CHARMS DATE: 2/25/93 CREATED BY USER: nauss 1639 0.00000 1 ILE -53.41835 ~52.87964 96.86949 A1 1 13 2 1 ILE HT1 -54.06550 -53.37379 96.22549 A1 0.00000 3 1 ILE -52.48505 -53.33354 0.00000 HT2 96.89426 A1 1 ILE HT3 -53.81151 -52.85195 97.84341 A1 0.00000 1 ILE -53.29159 -51.45945 96.52548 A1 CA 1 6 1 ILE CB -54.51076 -51.09296 95.64551 A1 0.00000 7 1 ILE -55.84867 -51.39510 0.00000 CG2 96.33544 A1 8 1 ILE CG1 -54.43380 -49.65164 95.12978 A1 0.00000 0.00000 9 1 ILE -55.55018 -49.30658 CD 94.14124 A1 10 -53.31306 -50.79352 0.00000 1 ILE С 97.88119 A1 1 0.00000 11 1 ILE 0 -53.76732 -51.45486 98.80800 Al 1 12 2 LYS -52,70566 -49,57271 97.98462 A1 2 0.00000 13 2 LYS -52,43149 -49,07042 0.00000. 11 97.19065 A1 14 2 LYS -52.72856 -48.82990 99.24363 A1 0.00000 Cλ 15 2 7,75 0.00000 -51.40674 -49.22996 100.05168 A1 2 CB 16 2 LYS 0.00000 "-51.65942 -50.46422 100.94226 A1 CG 2 0.00000 17 2 LYS CD -50.39491 -50.76541 101.74483 Al 2 18 2 LYS CE -50.65567 -51.67024 102.94896 A1 2 0.00000 19 -49, 48784--51.62033 103.84066 Al 0.00000 ,2 LYS NZ 20 2 LYS 1121 -49.68891 -52.15413 104.71032 A1 0.00000 -48.66152 -52.03086 103.36162 A1 2 LYS 122 0.00000 2 -49.28787 -50.62863 104.08530 Al 2 LYS H23 0.00000 2 23 2 LYS C -52.50080 -47.37619 98.85749 Al 2 0.00000 ·24 25 97.74074 23 2 LYS ٥ -52.16561 -47.08993 0.00000 3 GLU N -52.93375 -46.48610 0.00000 99.78817 A1 26 3 GLU H -53.25920 -46.74733 100.69754 A1 0.00000 27 3 GLU CA -52.88416 -45.05669 99.49342 A1 3 0.00000 28 3 GLU CB -54.17633 -44.67728 98.75869 Al 0.00000 -54.16941 -43.30721 -55.38365 -43.14982 29 3 GLU 0.00000 CG 98.07127 A1 3 30 3 GLU CD 97.16830 A1 3 0.00000 31 3 GLU -55.40070 -42.20412 -56.30088 -43.96983 OE1 96.38367 A1 3 0.00000 32 3 GLU OE2 97.23742 21 3 0.00000 33 3 GLU С ~52.73723 -44.30588 100.80334 A1 0.00000 34 3 GLU 0 -53.13310 -44.80289 101.85375 A1 0.00000 35 -52.10513 -43.13147 100.72198 A1 4 GLU N 0.00000 4 GLU 36 H -51.89913 -42.70887 99.83885 A1 0.00000 37 -51.71490 -42.41569 101.93532 A1 CA 0.00000 38 4 GLU CB -50.23606 -42.65775 102.23912 A1 0.00000 4 GLU CG -49.88908 -44.07273 102.69972 A1 0.00000 40 4 GLU CD -48.39447 -44.20822 102.86978 A1 0.00000 41 4 GLU OE1 -47.71593 -43.20739 103.12446 A1 0.00000 42 43 4 GLU OE2 -47.87485 -45.31826 102.72475 A1 0.00000 4 GLU С -51.86859 -40.92476 101.75610 A1 0.00000 44 4 GLU ٥ -51.85445 -40.40438 100.64776 A1 0.00000 5 HIS 45 -51.98758 -40.25490 102.89941 A1 -51.95529 -40.74179 103.77267 A1 N 5 0.00000 ٤6 н. 0.00000 47 5 HIS CA -52.02510 -38.79739 102.88794 A1 0.00000 5 HIS CB -52.95268 -38.30654 104.00423 A1 5 0.00000 49 5 HIS CG -54.39292 -38.58657 103.64511 A1 0.00000 50 5 HIS NDI -55.01336 -38.04007 102.58631 A1 0.00000 51 -54.63216 -37.40030 101.93314 A1 5 HIS HD1 0.00000 52 5 HIS -55.29163 -39.42491 104.31043 A1 CD2 0.00000 -56.46563 -39.37373 103.63249 A1 5 HIS NE2 0.00000 5 HIS CEL -56.29489 -38.51954 102.57197 A1 0.00000 5 HIS С -50.64149 -36.20241 103.06558 A1 0.00000 5 HIS 0 -49.75908 -38.78174 103.68940 A1 0.00000 6 VAL 1; -50.46014 -37.02655 102.46317 A1 0.00000 6 MAL H -51,22869 -36,59864 101,97707 A1 0.00000 6 VAL CA -49.12695 -36.41474 102.46426 A1 0.00000 -48.60121 -36.33669 101.01420 A1 5 MAI. CB 0.00000

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63	6 VA3	. cga	-47.0	2 -36.3011	9 101.00126	A1	6 0.00000
€2	6 VA				7 100.11057		6 0.00000
63	6 VAI	-			0 103.02675		6 0.00000
64	6 VAI				1 102.87457		6 0.00000
65	7 115				0 103.65431		7 0.00000
66	7 ILE	н	-47.3597	2 -35.1314	8 103.91409	λl	7 0.00000
67	7 ILE	CA	-48.0950	6 -33.0869	7 103.98819	λl	7 0.00000
68	7 ILE		-48.6919	7 <b>-</b> 32.8681	3 105.39701		7 0.00000
69	7 ILE				7 106.43001		7 0.00000
70	7 ILE				5 105.81727		7 0.00000
71	7 ILE				107.23523		7 0.00000
72	7 ILE	С			103.87753		7 0.00000
73	7 ILE	0		5 -33.1010			7 0.00000
74	8 ILE	И			103.23109		8 0.00000
75	8 ILE	Н		-30.79777			8 0.00000
76 77	8 ILE	CA			102.75879		8 0.000 <del>0</del> 0
78	8 ILE	CB			101.24826		8 0.00000
79	8 ILE	CGS			100.47371		8 0.00000 8 0.00000
80		CGI			100.51961		8 0.00000 8 0.00000
81	8 ILE	C			103.03239		8 0.00000
82	9 ILE	Ö			102.63903		8 0.00000
83	9 GLN	พ			103.70229		9 0.00000
84	9 GLN	H			104.05676		9 0.00000
85	9 GLN	CA			103.71549		9 0.00000
8.5	9 GLN	CB	_	-27.43231			9 0.00000
€7	9 GLN	CG		-27.13894		A1 !	9 0.00000
<b>6</b> 5	9 GLN	CD		-26.69043			9 0.00000
89	9 GLN	OEl	-44.59992	-27.05224	108.31811	Al !	9 0.00000
90	9 GLN	NE2		-25.86874			9 0.00000
91	9 GLN				106.73881		9 0.00000
92 63	a CIN				108.41526		9 0.00000
93 94	9 GTN	Ç			102.89330		9 0.00000
95	9 GLN	0.		-28.56703			9 0.00000
96	10 ALA 10 ALA	n H		-26.84230 -26.24022			10 0.00000 10 0.00000
97	10 ALA	A.		-26.60034			10 0.00000 10 0.00000
98	10 ALA	CB		-26.95993	99.69281		0.00000
95	10 ALA	C			101.25674		0.00000
100	10 ALA	0		-24,24680			0.00000
101	ll Glu	12	-39.11637	-24.95043	101.08226		0.00000
102	ıï era	H	-38.51800	-25.72332	100.86462	A1 1	0.00000
203	JJ CTA	CA	-38,56697	-23.61077	101.26935	<u>ሕ</u> ጋ 1	0.00000
104	11 GLU	·CB		~23,62729			0.00000
105 106	11 GLU	CG		-24,15021	103.73032		0.00000
107	11 GLU	CD		-24.35236	104.86668		0.00000
108	11 GLU	0E1			105,87939		0.00000
109	11 GLU	OE2 C		-23.95826	104.74301 2		.1 0.00000
110	11 GLU	Ö	-37.17390		.99.37097		.1 0.00000 .1 0.00000
111	12 PHE	N	-37.86688		99.78525		.1 0.00000 .2 0.00000
112	12 PHE	н	-38.38856	-21.25141	100.37827	43 1	2 0.00000
113	12 PHE	CA	-37.20863	-21.33691	98.59813		2 0.00000
214	12 PHE	CB	-38.26225	-21.06791	97.51950		2 0.00000
115	12 PHE	CG	-37.93682		96.2766B 1		2 0.00000
116	12 PHE	CD1	-38.35291		96.17465		2 0.00000
117	12 PHE	CD2	-37.21678		95.22261		2 0.00000
118	12 PHE	CEI	-38.04712		95.01356	-	2 0.00000
119	12 PHE	CE2	-36.91098		94.06122 /		2 0.00000
121	12 PHE	CZ	-37.32685		93.96022		2 0.00000
123	12 PHE	C	-36.45949		98.90209 3		
123	12 PRE	i1 O	-37.00216 -35.16677		98.93077 <i>3</i> 99.15293 <i>3</i>		
124	13 778	H	-34.71888	-21 10005	99.03346 /		3 0.00000
		••	57.72000	44.10000	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	•4 •	3 0.00000

FIG. 3

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125	13 TYR	CA	-34.44	-19.02891			13	7.00000
126	13 TYR	CB			1 100.90471		13	J.00000
127	13 7YR	ÇG		-18.04844		_	13	0.00000 0.00000
128	13 TYR	CD1		-17.52707			13	0.00000
129	13 TYR	CE1		-16.35710			13 13	0.00000
130	13 TYR	CD2		-17.40687			13	0.00000
131.	13 TYR	CE2		-16.23332			13	0.00000
132	13 TYR	CZ		-15.71594			13	0.00000
133	13 TYR	ОН		-14.58930			13	0.00000
134	13 TYR	нн	-	-14.89238			13	0.00000
135	13 TYR	C		-18.52544			13	0.00000
136	13 TYR	0		-19.23915 -17.25550			14	0.00000
137 138	14 LEU 14 LEU	И Н		-16.68306			14	0.00000
139	14 LEU	ÇA		-16.70428			14	0.00000
140	14 LEU	CB		-16.21044			14	0.00000€
141	14 LEU	CG		-17.29674			14	- 0.00000
142	14 LEU	CD1		-16.92524		λ1	14	0.00000
143	14 LEU	CD2	-32.72461	-17.54798	94.13078	λl	14	0.00000
244	14 LEU	c	-31.93377	-15.56813	97.60481	A1	3 4	0.00000
145	14 LEU	0	-32.31049	-14.71998			14	0.00000
146	15 ASN	N		-15.58168			15	0.00000
247	15 ASK	H		,-16.38705			15	0.00000
148	15 ASN	CA		-14.39297			15	0.00000 0.00000
149	15 ASK	CB		-14.93729			15	0.00000
150	15 ASN	CG		-14.18957	98.46652		15 15	0.00000
151	15 ASN	OD1 ND2		-13.98878 -13.74712	99.50693		15	0.00000
152 153	15 ASN 15 ASN	HD21		-13.93409			15	0.00000
154	15 ASN	HD22		-13.18778	98.98020		15	0.00000
155	15 ASI;	C		-13.70870			15	0.00000
156	15 ASN	Ö		-14.17939	94.92357		15	0.00000
157	16 PRO	N		-12.64312	95.25454	Al	16	0.00000
158	16 PRO	CD		-12.14147	.93.88390	Al	16	0.00000
<b>159</b>	16 PRO	CA	-28.34388	-11.89943	96.02164	A1	16	0.00000
160	16 PRO	CB		-11.32145			16	0.00000
161	16 PRO	CC		-11.06430	93.72211		16	0.00000
1,52	16 PRO	С		-10.84560	96.98393		16	0.00000
163	16 PRO	0		-10.81095	98.14625		16	0.00000
164	.7 ASP	N	-29.73099	9.96981	96.45979		17	0.00000
165 166	17 ASP 17 ASP	H.	-30.06531 -30.07647	-10.06794	95.52595 97.18869		17 17	0.00000
167	17 ASP	CA CB	-30.80318	-8.75629 -7.83976	96.20071		17	0.00000
168	17 ASP	CG	-30.22601	-6.44601	96.27578		17	0.00000
169	17 ASP	OD1	-29.42577	~6.10216	95.40955		17	0.00000
170	17 ASP	OD2	-30.58500	-5.71147	97.19272		17	0.00000
171	17 ASP	С	-30.91226	-8.96778	98.44177	Al	17	0.00000
172	17 ASP	٥.	-30.52677	-8.65960	99.56331		17	0.00000
173	18 GTM	N .	-32.11780	-9.49744	98.20428		18	0.00000
174	18 GLN	Н :	-32,36542	-9.81984	97.29256		18	0.00000
175 176	18 GLN	CŸ	-33.10696	-9.57864	99.27949		18	0.00000
177	18 GLN	СЭ	-34.05728	-8.37464	99.14180		18	0.00000
178	18 GLN	CĞ	-33.36307	-7.07517	99.58476		18 18	0.00000
179	18 GLN	CD OF1	-33.97880 -35.13776	-5.85158 -5.50918	98.94046 99.12725		18	0.00000
160	18 GLN	OE1 NE2	-33.14378	-5.16835	98.16624		18	0.00000
181	18 GLN		-32.19859	-5.47544	97.99847		18	0.00000
182	18 GLN		-33.43475	-4.32502	97.72302		18	0.00000
183	18 GLN	C		-10.91598	99.26964		18	0.00000
184	18 GLN	0	-33.74750	-11.68763	98.32391		18	0.00000
185	19 SER	11	-34.51482	-11.16924	100.39831		19	0.00000
186	19 SER	Я	-34.63228	-10.43617	101.06649	A1	19	0.00000
167	19 SER	CA	-34.94474	-12.50616	100.83625	Al	19	0.00000
188	19 \$ER	CB	-35.43672	-12.36114	102.28173	Αl	19	0.00000

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							19	0.00000
.189	19 SER				103.10841 103.40254		19	0.00000
190 191	19 SER 19 SER	нс С			100.02197		19	0.00000
192	19 SER	Ö		-12.86400			19	0.00000
193	20 GLY	N			100.53004		20	0.00000
194	20 GLY	H			101.41380		20	0.00000
195	20 GLY	CA		-15.47533			20	0.00000
196	20 GLY	C			100.44590		20	0.00000
197	20 GLY	0	-39.10838	-15.10421	101.05171	λl	20	0.00000
198	21 GLU	N	-38.72023	-17.18722	100.25477	λ1	21	0.00000
199	21 GLU	H	-38.03254	-17.84573	99.94375	λl	21	0.00000
200	21 GLU	CA	-40.11538	-17.64629	100.27114		21	0.00000
201	21 GLU	CB		-17.64420			21	0.00000
202	21 GLU	ÇG		-17.90322			21	0.00000
203	21 GLU	CD		-17.98331			21	0.00000
204	21 GLU	OE1		-17.59671			21	0.00000
205	21 GLU	OE2		-18.43207			21	0.00000~
206	21 GLU	С			100.89226		21 21	0.00000
207	21 GLU	0			101.07437		22	0.00000
208 209	22 PHE 22 PHE	н	-41.54286		101.01655		22	0.00000
210	22 PHE	CA			101.93252		22	0.00000
-211	22 PHE	CB			103.43794		22	0.00000
212	22 PHE	CG	-41,45246	-21.48591	104.34752	A1	22	0.00000
213	22 PHE	CD1	-40.59481	-21.25886	105.44915	Al	22	0.00000
214	22 PHE	CD2	-42.01384	-22.76966	104.14562	Al	22	0.00000
215	22 PHE	CEl	-40.30109	-22.30643	106.34948	Al	22	0.00000
216	22 PHE	CE2	-41.72224	-23.81970	105.04232	Al	22	0.00000
217	22 PHE	CZ	-40.86722	-23.58408	106.14281	A1	22	0.00000
218	22 PHE	С	-43.25845	-21.11988	101.58028	Al .	22	0.00000
219	22 PHE	٥	-44.19436	-20.32985	101.55111	X1	22	0.00000
220	23 MET	N	-43.39639	-22.43138	101.32298	VI	23 23	0.00000
221 222	23 MET 23 MET	H	-42.59132	-23.03279	101.30500	P.J	23	0.00000
223	23 MET 23 MET	CA CB		-22.73266			23	0.00000
224	23 MET	CG		-23.35273			23	0.00000
225	23 MET	SD		-23.10231			23	0.00000
226	23 MET	CE		-24.67640			23	0.00000
227	23 MET	Ċ			101.21411	A1	23	0.00000
228	23 MET	0			100.62115		23	0.00000
229	24 PHE	N			101.99622		24	0.00000
230	24 PHE	H			102.03772		24	0.00000
231	24 PHE	CA			102.69060		24	0.00000
232 233	24 PHE 24 PHE	CB			103.21139		24 24	0.00000
234	24 PHE	CD1			105.60532		24	0.00000
235	24 PHE	CD2			104.40480		24	0.00000
236	24 PHE	CEI			106.75356		24	0.00000
237	24 PHE	CE2			105.55271		24	0.00000
238	24 PHE	CZ	-44.89594	-22.39162	106.72434	A1	24	0.00000
239	24 PHE	C .	-47.88569	-25.61775	101.85776	Al	24	0.00000
240	24 PHE	0	-48.73152	-24.87778	101.36424	Al	24	0.00000
241	25 ASP	N	-47.89855	-26.94593	101.74049	A1	25	0.00000
242 243	25 ASP	H			102.20704		25	0.00000
244	25 ASP 25 ASP	CA CB		-27.84762	100.90165		25 25	0.00000 0.00000
245	25 ASP	CG		-28.30012	98.47932		25	0.00000
246	25 ASP	ODl		-27.46672	97.77589		25	0.00000
247	25 ASP	002		-29.50745	98.38197		25	0.00000
246	25 ASP	С	-49.18430	-28.98699	101.56183	Al	25	0.00000
249	25 ASP	0			102.56241		25	0.00000
250	26 PHE	11	-50.15819	-29.70261	101.00377	Αl	26	0.00000
251	26 PHE	H.			100.15349		26	0.00000
252	26 PHE	CA	-50.5603	-30.99701	101.54898	r. 1	26	0.00000

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							26 0.00000
253	26 PRE	CB			102.82009		
254	26 PHZ				102.57724		
255	26 PHE	CD1		-28.5567			
256	26 PHE	CD2			5 101.99011		
257	26 PHE	CE1			102.66706		
258	26 PHE	CE2		•	5 101.74257		
259	26 PHE	CZ		-28.18547			
260	26 PHE	С		-31.82500			26 0.00000
261	26 PHE	0		-31.38211			26 0.00000
262	27 ASP	N			100.89199		0.00000
263	27 ASP	H			101.83544		0.00000
264	27 ASP	CA		-34.11623			27 0.00000
265	27 ASP	CB		-34.25359			
266	27 ASP	CG		-35.66101			
267	27 ASP	001		-36.23164			
26B	27 ASP	OD2			100.47314		
269	27 ASP	Ç		-34.05698			
270	27 ASP	0		-34.)0386		-	
271	28 GLY	N		-33.92246			
272	28 GLY		·· -49.78144			_	
273 274	28 GLY	CA.		-33.86633			
	28 GLY	C		-32.51821			0.00000 8 0.00000
275 276	28 GLX	0		.,-32.03342			•
277	29 ASP	N		-31.96145			0.00000
276	29 ASP	H		-32.39453			9 0.00000
279	29 ASP	CX		-30.85124			9 0.00000
250	29 ASP 29 ASP	CB.		-31.44665 -30.54960			9 0.00000
281	29 ASP 29 ASP	CG OD1	-51 (3/20	-30.32445			9 0.00000
262	29 ASP	OD2	-53 56233	-30.10545	92.75048		9 0.00000
283	29 ASP	C		-29.64631			9 0.00000
284	29 ASP	ŏ		-28.59407			9 0.00000
285	30 GLU	N		-29.81701	97.32405		0.00000
286	30 GLU	н	•	-30.57647	97.90251		0.00000
287	30 GLU	CA		-28.70871			0.00000
288	30 GLU	CB		-29.18152			0.00000
239	30 GLU	CG		-29.71506		A1 3	0.00000
290	30 GLU	CD	-57.13279	-29.50058	98.43828	A1 3	0.00000
291	30 GLU	OE1		-30.47326		A1 3	0.00000
292	30 CTA	OE2	-57.48939	-28.34297	98.66447	A1 3	0.00000
293	30 Gru	С	-52.69655	-27.80995	98.82987	A1 3	0.00000
294	30 CTA	0	-52.13191	-28.20198	99.84476	λ1 3	0.00000
295	31 ILE	N		-26.53268	98.46810	A1 3	0.00000
296	31 ILE	. H	-53.28532	-26.29454	97.65353		0.00000
297	33 ILE	CA	-51.98442		99.18511		0.00000
298	31 ILE	CB	-51.81933		98.23317		0.00000
299	31 ILE	CG2	-53.16329		97.91607		1 0.00000
300	31 ILD	CG1	-50.75168		98.71478		1 0.00000
301	31 ILE	CD	-50.41981		97.66271		1 0.00000
302 303	31 ILE	C			100.56211		1 0.00000
304	31 ILE	0		-24.97567			1 0.00000
305	32 PHE	₩.			101.46562		
305	32 PHE 32 PHE	H			101.18020		
307	32 PHE	CA CB			102.84494		
308	32 PHE	CG			104.74893		
309	32 PHE	CD1			105.15120		
310	32 PHE	CD2	-52.49149				
311	32 PHS	CEI			106.12524		
312	32 PHE	CE2			106.29575		
313	32 PHE	ÇZ			106.69566		
314	32 PHE	c	-51.84397	-23.07181	103.07985	A1 3	2 0.00000
315	32 PHE	0	-52.76581	-22.45086	103.€2205	A1 3	
316	33 HIS	33	-50.69095	-22.50451	102.70813	A) 3	3 0.00000

FIG. 6

./၁೯:_1	KIN2.CHD		Thu Fab	25 14:58:4	8 1993		6	
317	SIK EE	H	-50.04	-22.98834	102.10786	A1	33	0.00000
318	33 HIS	Ĉλ	-50.22.		103.23242		33	0.00000
319	33 HIS	CB		-21.51540			33	0.00000
320	33 HIS	CG		-20.32142			33	0.00000
	33 HIS	ND1		-19.72793			33	0.00000
321	33 HIS	HD1	-47 20000	-19.92757	104 75923	A 1	33	0.00000
322	33 HIS		-40 07214	-19.68828	106.45019	λl	33	0.00000
323		CD2		-18.70682			33	0.00000
324	33 HIS	NE2		-18.72654			33	0.00000
325	33 HIS	CEI	40 31513	-20.78472	102 29629		33	0.00000
326	33 HIS	C	-49.11511	-21.61206	102.27025	B 1	33	0.00000
327	33 HIS	٥	-48.59725	-21.61206	101.55645	Al	34	0.00000
328	34 VAL	N	-48,74537	-19.50449	102.33033		34	0.00000
329	34 VAL	H	-49.19429	-18.80802	102.90163	V.T		0.00000
330	34 VAL	CA	-47.51776	-19.11490	101.64269	A1	34	0.00000
331	34 VAL	ĊВ		-18,42567			34	0.00000
332	34 VAL	CG1		-18.41158	99.39158		34	0.00000-
333	34 VAL	CG2	-48.95871	-19.06363	99,49806		34	
334	34 VAL	С	-46.79652	-18.14692	102.56509	Al	34	0.00000
335	34 VAL	0	-47.41849	-17.54298	103.42874	Al	34	0.00000
336	35 ASP	N	-45.47963	-18.03426	102.37666		35	0.00000
337	35 ASP	н	-45.03039	-18.68906	101.76710		35	0.00000
338	35 ASP	CA	-44.68799	-16.93300	102.93355	Αl	35	0.00000
.339	35 ASP	СВ	-4474876	-15.73492	101.94639	ħ1	35	0.00000
340	35 ASP	CG	-46.11850	-15.06364	101.88569	Al	35	0.00000
341	35 ASP	OD1	-46.85196	-15.31279	100.93528	A1	35	0.00000
342	35 ASP	CD2	-46.43780	-14.28565	102.78747	Αì	35	0.00000
343	35 ASP	c		-16.57120		Al	35	0.00000
344	35 ASP	õ		-17.43137		Al	35	0.00000
345	36 MET	N .	-44.91212	-15.26386		Al	36	0.00000
346	36 MET	н :	-44.97503	-14.58792	103,95356	A1	36	0.00000
347	36 MET	CA	-45.05621	-14.74244	106.04065	Al	36	0.00000
348	36 MET	CB		-13.28473		Al	36	0.00000
349	36 MET	ÇG.	-43.15122	-13.10955	105.50403	λl	36	0.00000
350	36 MET	SD.	-42 96722	-11.71848	104.37016	Al	36	0.00000
351	36 MET	CE		-10.40582		A1	36	0.00000
352	36 MET	6	-46 49207	-14.77022	106.53712	A.1	36	0.00000
353	36 MET	0		-14.73983		Al	36	0.00000
354	37 ALA	N		-14.78996		Al	37	0.00000
355	37 ALA	н		-14.87225		λl	37	0.00000
356	37 ALA	CA	-49 B0100	-14.57493	106.05297	Al	37	0.00000
357	37 ALA	CB		-13.19637		Al	37	0.00000
358	37 ALA	C		-15.61256		Al	37	0.00000
359	37 ALA	ō		-16.18787		A.1	37	0.00000
360	38 LYS	N		-15.79391		λl	38	0.00000
361	38 LYS			-15.37866		Al	38	0.00000
362	38 LYS	H CA		-16.48765		Al	38	0,00000
363	38 LYS			-16.55867		Al	38	0.00000
364	38 T.X2.	CB		-17.48517		λl	38	0,00000
365		CG	-52.91303	-18.62084	100.00230		38	0.00000
366	38 T.Z 38 T.Z	CD,	-53 42547	-19.66155	107 75111	λl	38	0.00000
367	38 LYS	CE ·		-20.17861			38	0.00000
368			-54.70303	-20.92377	107.50055	2.1	38	0.00000
369	38 LYS	1121	-54.79220	-20.59510	100.03733	14	38	0.00000
	38 LY5	HZ2	-52.17073	-20.33310	100.44040	2.1	38	0.00000
370	38 LYS	HZ3	-52.42/4/	-19.41621	105 12000			0.00000
371	38 LYS	C		-15:73437			38	0.00000
372	38 LYS	0	-52.72521	-14.51209	105.10297	V.	38	
373	33 LYS	N	-53.35457	-16.44351	104.17702	ĀΙ	39	0.00000
374	30 TAR	H	-53.59774	-15.96113	103.33578	A.	39	0.00000
375	39 LYS	CA	-53.67982	-17.86931	104.22041	A.	39	0.00000
376	39 LYS	CB	-55.18971	-18.00506	104.55346	Al	39	0.00000
377	39 LYS	CG	-56.24681	-17.84030	103.42417	Al.	39	0.00000
378	39 F.R	CD	-56.27039	-15.52580	102.62130	ΥŢ	39	0.00000
379	39 LYS	CΞ	-56,64532	-16,69161	101.13213	V.1	39	0.00003
380	39 1.75	NC.	-55.66137	-17 54662	100.43832	F. :	3 9	0.00000

./27:	_ಖರಗಿನ . ರಜ	<b>5</b>	Thu Fa	5 25 14:58	:48 1993	7	
381	39 LY	S HZ	1 <b>-5</b> 5.r	45 -18.5450	31 100.36313	A1 39	0.00000
382		5 H22	2 -55	63 -17.2672	25 99.46103	11 39	0.00000
383			3 -54.7241	36 -17.5192	21 100.90690	1 39	0.00000
384		C	-53.4442	23 -18.4428	3 102.84433 2	1 39	0.00000
385			-53.4335	51 -17.6751	8 101.88936 2	1 39	0.00000
386	40 GLU	N	-53.4133	32 -19.7742	0 102.71885 /	11 40	0.00000
387	40 GLU	H	-53.1615	64 -20.4369	1 103.42697 /	1 40	0.00000
388	40 GLU	CA	-54.0889	2 -20.1464	5 101.48663 /	1 40	0.00000
389	40 GLU				3 100.44056 7		0.00000
390	40 GLU			3 -19.8275			0.00000
391	40 GLU			7 -18.9010			0.00000
392	40 GLU			1 -17.6837			0.00000
393	40 GLU			6 - 19.3556			0.00000
394	40 GLU				6 101.61501 A		0.00000
395	40 GLU	0			4 101.08479 A		0.00000
396	41 THR	N			6 102.35754 A		0.00000
397	41 THR	11			2 102.86321 A		0.00000
398	41 THR	CA		6 -22.5546			0.00000
399 400	41 THR	CB		1 -24.0583			0.00000
401	41 THR	0G1		2 -24.7540			0.00000
402	41 THR	HG1 CG2		5 -25.5961			0.00000
.403	41 THR	C		4 -24.6717; 2 -22.26510			0.00000
404	41 THR	0		7 -21.9354			0.00000
405	12 VAL	N		6 -22.4152			0.00000
406	42 VAL	я		7 -22.8142			0.00000
407	42 VAL	CA			1 103.80812 A		0.00000
408	42 VAL	CB			6 102.98525 A		0.00000
409	42 YAL	CG1			103.74041 A		0.00000
410	42 VAL	CG2			3 101.63610 A		0.00000
411	42 VAL	С			105.14170 A		0.00000
412	42 VAL	٥			106.20404 A		0.00000
413	43 TRP	N·	-60.26652	-24.07997	7 105.07466 A	1 43	0.00000
414	43 TRP	н.	-60.09540	-24.53437	1 104.20145 A	1 43	0.00000
415	43 TRP	CA	-60.35176	3 -24.82113	3 106.34002 A	1 43	0.00000
416	43 TRP	CB.	-60.91225	-26.25321	. 106.17013 A	1 43	0.00000
417	43 TRP	CG	-60.96314	-26.72686	104.73262 A	43	0.00000
310	43 TRP	CD2			103.92127 A		0.00000
419 420	43 TRP	CE2		-27.49629			0.00000
421	43 TRP 43 TRP	CE3	-58.50029				0.00000
422	43 TRP	CD1 NE1	-62.11826	-26.86040	103.93459 A	43	0.00000
423	43 TRP	HEL	-61.841/4	-27.31306	102.67766 AT	43	0.00000
424	43 TRP	CZ2			101.58525 Al		0.00000
425	43 TRP	CZ3	-57.69263	-27.72260	103.07694 A1	43	0.00000
426	43 TRP	CH2	-58.24204	-28.07937	101.82597 A	43	0.00000
427	43 TRP	c.	-59.07150	-24.84373	107.16564 A1	43	0.00000
428	43 TRP	0	-58.85050	-25.68073	108.02836 A1		0.00000
429	45 ARG	N	-58.22471	-23.84563	106.89519 A1	44	0.00000
430	44 ARG	H	-58.31398	-23.27977	106.07364 A1	44	0.00000
431	44 ARG	CA	-57,22046	-23.49560	107.89144 A1	44	0.00000
432	44 ARG	CB	-55.83244	-23.69727	107.26013 A1	44	0.00000
433	44 ARG	CG	-54.63741	-23.63473	108.22026 A1	44	0.00000
434	44 ARG	CD	-53.30915	-23,64273	107,47006 A1	44	0.00000
435	44 ARG	NE	-52.18625	-23.26000	108.32672 A1	44	0.00000
436	44 ARG	HE	-52.36221	-22.91543	109.25139 A1	4.4	0.00000
437 438	44 ARG	CZ			107.86475 A1	44	0.00000
439	44 ARG	NHl			108.56844 A1	4.4	0.00000
440	44 ARG	HH11		-22.84912	108.24673 A1	44	0.00000
441		NH2	-50.05182		109.51721 A1	44	0.00000
442	44 ARG		-49.73591		106.69352 A1 106.35139 A1	44	0.00000
443			-51 41740	-23.50000	106.35139 A1	4 4 4 4	0.00000
444	44 ARG	C	-57.42751	-22.05857	108 38029 A1	44	0.00000
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FIG. 8

਼./ਪਨ1_	אבווי2.כזים		Thu Feb	25 14:58:4	8 1993		8	
445	44 ARG	0	-56.5	-21.39201	108.88943	<b>A1</b>	44	0.00000
446	45 LEU	11	-58.65470	-21.55686	108.18548	λl	45	0.00000
447	45 LEU	H	-59.36846	-22.06382	107.69729	λl	45	0.00000
448	45 LEU	CA	-58.94679	-20.21897	108.70611	λl	45	0.00000
449	45 LEU	CB	-59.87267	-19.46515	107.74942	γī	45	0.00000
450	45 LEU	CG	-59:15056	-18.96990	106.49579	A1	45 45	0.00000
451	45 LEU	CD1	-60.14534	-10.41900	105.47407 106.87944	71	45	0.00000
452	45 LEU	CD2	-58.10431	-20 20104	110.09168	A)	45	0.00000
453 454	45 LEU 45 LEU	C O	-59.55616	-10 19926	110.79199	A1	45	0.00000
455	46 GLU	и	-59.33302 -60 08017	-21 36024	110.48954	λl	46	0.00000
456	46 GLU	н.	-60.14047	-22.14708	109.87631	λ1	46	0.00000
457	46 GLU	CA	-60.58379	-21.47317	111.86481	Al	46	0.00000
458	46 GLU	CB	-61.47817	-22.71518	111.95437	<b>л</b> 1	. 46	0.00000
459	46 GLU	CG			111.51772		46	0.00000
460	46 GLU	CD			111.46594		46	0.00000
461	46 GLU	OE1			110.36424		46	0.00000
462	46 GLU	OE2			112.52280		46 46	0.00000
463 464	46 GLU 46 GLU	.o			112.92683		46	0.00000
465	47 GLU	N			112.44220		47	0.00000
466	47 GLU	н			111.48920		47	0.00000
.467	47 GLU	CA			113.27698		47	0.00000
468	47 GLU	CB			112.39059		47	0.00000
469	47 GLU	CG	-55.95036	-23.50661	111.78977	A2	47	0.00000
470	47 GLU	CD			112.78701		47	0.00000
471	47 GLU	OE1			112.37878		47	0.00000
472	47 GLU	OE2			113.95212		47	0.00000
473 474	47 GLU 47 GLU	C			113.91510 113.26194		47 47	0.00000
475	48 PHE	0			115.24713		48	0.00000
476	48 PHE	ä			115.72305		48	0.00000
477	48 PHE	C.Y.	-56.75617	-19.13647	115.96362	Al	48	0.00000
478	48 PHE	CB	-57.20231	-19.34982	117.41420	Al	48	0.00000
479	48 PHE	CG			117.70829		4 B	0.00000
480	48 PHE	CD1			117.44215		48	0.00000
461 482	48 PHE	CD2			118.24455		48 48	0.00000
483	48 PHE	CE1 CE2			117.71246 118.51469		48	0.00000
484	48 PHE	CZ			118.24779		48	0.00000
485	48 PHE	c			115.93777		4.8	0.00000
486	48 PHE	0			115.72587		48	0.00000
487	49 GLY	ĸ			116.19761		49	0.00000
488	49 GLY	н			116.34575		49	0.00000
489	49 GLY	CV		.,	116.13162		49	0.00000
490	49 GLY	C			116.68056		49	0.00000
491 492	49 GLY 50 ARG	0			116.10714		49 50	0.00000
493	50 ARG	N. H			117.81779		50	0.00000
494	50 ARG	CA			118.42224		50	0.00000
495	50 ARG	CB	-52,27437	-18.92760	119.68340	Al	50	0.00000
496	50 ARG	CG	-51.10260	-19.32736	120.58254	Al	50	0.00000
497	50 ARG	CD	-53.53002	-20.14774	121.80047	λl	50	0.00000
498	50 ARG	NE			122.64580		50	0.00000
499 500	50 ARG	HE	-49.69865	-19.71957	122.75767	Al .	50	0.00000
500 501	50 ARG 50 ARG	C2			123.26571 124.04503		50 50	0.00000
502	50 ARG	6877 887			124.04503		50	0.00000
503	50 ARG				124.16453		50	0.00000
504	50 ARG	N∺2			123.10623		50	0.00000
505	50 ARG	HH21	-51.08073	-23.47414	123.56513	Al	50	0.00000
506	50 ARG				122.51852		50	0.00000
507	50 ARG	С	-51.06703	-19.09581	117.49074	۸ <u>:</u>	50	0.00000
508	50 ARG	o	-49.84240	-19.09133	117.41926	F	50	0.00000

נגכ/.	_KIN2.CRD	ı	Thu Isd	25 14:58:	48 1993	9	
509	51 PHE	N	-51.84	-19.8777	8 116.73839	A1 51	C.00000
510				4 -19.7665	7 116.76797		0.00000
511	51 PHE	CA	-51.2947	7 -20.7879	6 115,73402	λ1 51	0.00000
512		CB			3 115.15449		0.00000
513	51 PHE	CG			4 114.02359		0.00000
514	51 PHE	CD1			1 114.29503		0.00000
515	51 PHE	CD2			4 112.69289		0.00000
516	51 PHE	CEI					D.00000
517	51 PHE	CE2			1 113.22969		0.00000
					2 111.63059	_	0.00000
518	51 PHE	CZ			0 111.90000		
519	51 PHE	C			6 114.69371		0.00000
520	51 PHE	0			1 114.47961		0.00000
521	52 ALA	א			2 114.10202		0.00000
522	52 ALA	Н			114.33870		0.00000
523	52 ALA	CA			5 113.11957		0.00000 🛳
524	52 ALA	CB			5 112.62511		0.00000 -
525	52 ALA	С	-49.28257	-17.48933	3 113.62687	A1 52	0.00000
526	52 ALA	0			112.94510		0.00000
527	53 SER	N			114.88764		0.00000
528	53 SER	н	·· -50.22411	-17.11498	115.38567	41 53	0.00000
529	53 SER	CA	-48.18100	-16.47055	115.53815	41 53	0.00000
530	53 SER	CB	-48.58146	-16.02158	116.95383	11 53	0.00000
531	53 SER	OG	-47.59593	-15.15541	117.52845 /	1 53	0.00000
532	53 SER	HG			118.42105		0.00000
533	53 \$ER	c	-46.99433	-17.42737	115.57426		0.00000
534	53 SER	0			115.12568		0.00000
535	S4 PHE	и.			116.08200 2		0.00000
536	54 PHE	بر			116.41568 /		0.00000
537	54 PHE	CA			116.09999 2		0.00000
538	54 PHE	CB.			116.63413 #		0.00000
539	54 PHE	CG			118.13255 2		0.00000
540	54 PHE	CD1			118.65539 #		0.00000
541	54 PHE	CD2			119.00621 #		0.00000
542	54 PHE	CEl			120.05266		0.00000
543	54 PHE	CE2			120.40382 2		0.00000
544	54 PHE	CZ			120.92307 A		0.00000
545	54 PHE	С			114.73758 A		0.00000
545	54 PHE	0			114.55246 A		0.00000
547	55 GLU	N			113.76558 A		0.00000
548	55 GLU	H,	-47.45338	-20.04226	113.95516 A	1 55	0.00000
5,49	55 GLU	CA			112.42886 A		0.00000
550	55 GLU	CB	-47.14512	-20.81915	111.54876 A	1 55	0.00000
551	55 GLU	CG	-47.92567	-21.96126	112.19274 A	1 55	0.00000
552	55 GLU	.CD	-49.04456	-22,36202	111.27677 A	1 55	0.00000
\$53	55 GLU	OE1	-49.15553	-23.53977	110.96047 A	1 55	0.00000
554		OE2	-49.80524	-21.50984	110.81474 A	1 55	0.00000
\$55		C.	-45.19354	-19.30188	111.76318 A	1 55	0.00000
5.5.6	55 GLU	oʻ	-44.12678	-19.50387	111.19343 A	1 55	0.00000
\$57		N	-45.73650	-18.08673	111.89532 A	1 56	0.00000
558	56 ALA	X	-46.62336	-17,96765	112.34890 A	1 56	0.00000
559	56 ALA	CA			111.38640 A		0.00000
560	56 Ala	CB	-45.80074	-15.63871	111.59969 A	56	0.00000
561	56 ALA	С	-43.63772	-16.77849	112.02791 A	56	0.00000
562	56 ALA 6	0			111.36878 A		0.00000
563		N			113.35929 A		0.00000
564	57 GLN 1	H	-44.48826 -	-17.03983	113.86832 A	57	0.00000
565		Cλ	-42.35063 •	-16.88200	114.06847 A	57	0.00000
566		CB	-42,61987 -	-17.03049	115.56930 A	57	0.00000
567		CG			116.45895 A		0.00000
565		CD			117.90800 A		0.00000
569		DE1	-42,29879 -	-16.06206	118.58910 A	57	0.00000
570		NE2			116.38366 AT		0.00000
571			-41.14709 -	18.27176	117.81428 A	57	0.00000
572	57 GLN 1	FE22	-41.78115 -	18.36728	119.33313 A	57	0.00000
							4.44000

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573	S7 GLN	c -41. i3 -17.94055 l	13.59025 Al	57	0.00000
574	57 GLN	C -41. 13 -17.94055 1 O -40.18971 -17.68051 1	13.34773 AL	57	0.00000
575	58 GLY	N -41.88825 -19.15742 1	13.41319 Al	58	0.00000
576	58 GLY	H -42.84771 -19.33514 1	13.64847 Al	58	0.00000
577	58 GLY	CA -41.05379 -20.23393 1	12.87374 A1	58	0.00000
578	58 GLY	C -40.45534 -19.92781 1	11.50957 Al	58	0.00000
579	58 GLY	0 -39.25324 -20.01021 1	11.27849 Al	58	0.00000
580	59 ALA	N -41.34654 -19.52227 1	10.60018 A1	59	0.00000
581	59 ALA	H -42,32072 -19.46762 1	10.83485 Al	59	0.00000
582	59 ALA	CA -40.88666 -19.14537 1	09.26181 31	59	0.00000
583	59 ALA	CB -42.07124 -18.74086 1	08.38101 A1	59	0.00000
	59 ALA	C -39.86090 -18.02257 1	09.26073 A1	59	0.00000
584 585	59 ALA	0 -38.85187 -18.04905 1	08.56603 A1	59	0.00000
_	60 LEU	N -40.12979 -17.02925 1	10.11113 A1	60	0.00000
586 587	60 LEU	H -40.96678 -17.03715 1	10.66448 Al	60	0.00000
588	60 LEU	CA -39.17026 -15.93079 1	10.21454 31	60	0.0000
589	50 LEU	CB -39.62974 -14.72108 1	10.88234 A1	60	0.00000
590	60 TEA	CG -41.00342 -14.16448 1	10.06267 A1	60	0.00000
591	60 LEU	CD1 -41.72077 -13.05637 1	10.83175 Al	60	0.00000
592	60 LEU	CD2 40.54968 -13.69403-1	08.67852 Al	60	0.00000
593	60 LEU	C -37.86300 -16.28607 1	10.90549 Al	60	0.00000
594	60 LEU	0 -36,81366 -15,71151 1	10.64266 Al	60	0.00000
595	61 ALA	N -37.92548.+17.30628.1	11.76650 Al	61	0.00000
596	61 ALA	H -38.80(16 -17.70206 1	12.04737 Al	61	0.00000
597	61 ALA	CA -36,66060 -17,86080 1	12.25036 A1	61	0.00000
59€	61 ALA	CB -36.90091 -18.87147 1	13.37402 Al	61	0.00000
599	61 ALA	c -35,86652 -18,52303 1	11.13575 Al	61	0.00000
600		0 -34 67753 -18.28483 1	10.93578 Al	61	0.00000
601	62 ASN	N -36.59182 -19.33811 1	10.35468 Al	62	0.00000
602	62 ASN		10.56458 AL	62	0.00000
603	62 ASN	CA -35.93048 -19.97053 1	09.20954 Al	62	0.00000
604	62 ASN	CB -36.90608 -20.83397 1	08.41185 Al	62	0.00000
605	62 ASN	CG -36.14296 -21.97501 1	07.76767 A1	62	0.00000
606	62 ASN	OD1 -35.90083 -23.00051 1	08.38915 Al	62	0.00000
607	62 ASN		06.49294 Al	62	0.00000
608	62 ASN	HD21 -35.71613 -20.90910 1	06.04169 AL	62	0.00000
609	62 ASN		05.92778 A1 08.27635 A1	62 62	0.00000
610	62 ASN			62	0.00000
611	62 ASN		07.30073 81	63	0.00000
612	63 ILE		07.31224 A1	63	0.00000
613 614	63 ILE 63 ILE		07 05550 31	63	0.00000
615	63 ILE	CA -35.60960 -16.86395 1 CB -36.79680 -15.88630 1		63	0.00000
616	63 ILE	CG2 -36.71800 -14.58751 1		63	0.00000
617	63 ILE	CG1 -37.00443 -15.60068 1	05.36486 Al	63	0.00000
618	63 ILE	CD -38.27181 -14.79756 1	05.06416 Al	63	0.00000
619	63 ILE	C -34.32421 -16.14412 1	07.48562 A1	63	0.00000
620	63 ILE	0 -33.67028 -15.43835 1	06.72047 Al	63	0.00000
621	64 ALA	N -33 97867 -16.34078 1	08.76481 A1	64	0.00000
622	64 ALA	н -34.55914 -16.88095 1	09.37800 Al	64	0.00000
623	64 ALA	CA -32.68252 -15.86370 1	09.23001 Al	64	0.00000
624	64 ALA	CB -32.78414 -15.37252 1	10.67448 %1	64	0.00000
625	64 ALA	C -31.59324 -16.91956 1	09.13883 Al	64	0.00000
626	64 ALA	0 -30.45701 -16.65389 1	08.75412 Al	64	0.00000
627	65 VAL	N -31.96250 -18.15367 1	09.50633 A1	65	0.00000
628	65 VAL	н -32.92093 -18.37377 1	09.71401 Al	65	0.00000
629	65 VAL	CA -30.91507 -19.17596 1	09.47932 Al	65	0.00000
630	65 VAL	CB -31.28412 -20.41152 1	10.33210 Al	65 65	0.00000
631	65 VAL		11.77524 61	65 65	0.00000
632	65 VAL	CG2, -32.45603 -21.23819 1	74 CCC30 41	65	0.00000
633	65 VAL	C -30.45713 -19.56758 1 O -29.26568 -19.71596 1	00.00237 AZ	65	0.00000
634 635	65 VAL		07.15805 21	66	0.00000
636	66 ASP 66 ASP	N -31.42136 -19.66037 1 E -32.38553 -19.49723 1	07.38832 A1	6.5	0.00000

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63,7	66 ASP	CA	-31.0. 3	-19.93216	105.76795	A1	66	0.00000
638	66 ASP	CB	-32.31036	-20.24966	104.93007	7.7	66 66	0.00000 0.00000
639	66 AŞP	CG	-33.44297	-19.24219	105.08208	Al El	66	0.00000
640	66 ASP	ODl	-33.16986 -34.60286	-18.05114	105.20729	λl	66	0.00000
641 642	66 ASP 66 ASP	OD2 C	-30 18178	-18.83449	105.15564	λl	66	0.00000
643	66 ASP	Ö	-29.16482		104.50705	λl	66	0.00000
644	67 LYS	N	-30.56424		105.48017	A1	67	0.00000
645	67 LYS	H	-31.49538			λı	67	0.00000 0.00000
646	67 LYS	CY	-29.72959	-16.43204	105.19320		67 67	0.00000
647	67 LYS	СВ	-30.39071	-15.23196	105.87104	NI NI	67	0.00000
648	67 LYS	ÇG	-29.79159 -30.51506	-13.86177	106.38164	31	67	0.00000
649 650	67 LYS 67 LYS	CD CE	-29.96446		106.14720		67	0.00000
651	67 LYS	NZ	-30.60526		107.01869		67	0.00000
652	67 LYS	HZl	-30.33262	-9.48398	106.85909		67	0.00000
653	67 LYS	HZ2	-31.70143			<b>X1</b>	67	0.00000
654	67 LYS	HZ3	-30.53221			Y]	67 67	0.00000
655	67 LYS	C	-28.28117	-16.58093	105.64383		67	0.00000
656 657	67 LYS 68 ALA	N	-28.12520	-16.92373			68	0.00000
658	68 XLX	н	-28.92119	-17.00935	107.53692	27	68	0.00000
659	68 ALA	CA	-26.76352	-17.18143	107.40958	λl	68	0.00000
660	68 ALA	CB	-26.77377	-17.44846		A1	68	0.00000
661	ALA 86	C	-26.07149	-16.34364		A1	68	0.00000
662	68 ALA	0	-24,80989				68 69	0.00000
. 663	69 ASN	×	-26.87877 -27.84416		106.44973	λì	69	0.00000
664 665	RZA 69 NZA 69	H Ca	-26.32826		105.77098	77	69	0.00000
666	69 ASN	CB	-27.33794		105.74618	Al	69	0.00000
667	69 ASK	CG	-27.75534	-22.20215	107.12937		69	0.00000
668	69 ASN	OD1	-28.81753	-22.77967	107.30600		69	0.00000
669	69 ASN	ND2	-26.90880		108.13718	Al	69	0.00000
670	69 ASN	HD21	-26.02949	-21.53117	108.03476	Al Al	69 69	0.00000
671	69 ASN 69 ASN	HD22 C	-27.17968 -25.83413		104.36379		69	0.00000
672 673	69 ASN	0		-20.87816			69	0.00000
674	70 LEU	N	-26.46696	-19.27268	103.71664	Al	70	0.00000
675	70 LEU	н		-18.83110	104.12686	Al	70	0.00000
676	70 LEU	CA		-18.80513			70 70	0.00000
677	70 LEU	CB		-17.57714	101.93156		70	0.00000
678 679	70 LEU 70 LEU	CG CD1	-28.07464 -28.90878			A1	70	0.00000
680	70 LEU	CD2		-18.56192	99.96378		70	0.00000
681	70 LEU	C		-18.42736			70	0.00000
682	70 LEU	0		-18.86456			70	0.00000
683	71 GLU	N	-24.17065		103.54240		71	0.00000
684	71 GLU	H	-24.87529 -22.77364	-17.33320	104.19342	Al Al	71 71	0.00000
685 686	71 GLU 71 GLU	CB CB	-22,71304	-16.23884			71	0.00000
€87	71 GLU	CG	-21.33647	-15.50613		Al	71	0.00000
883	71 GLU	CD	-21.30052	-14.53829	106.10023	λl	71	0.0000
689	71 GLU	OEl	-20.27115	-14.47665	106.76970	YJ	71	0.00000
€90	71 GLU	OE2	-22.29376	-13.85012	106.33423	A1	71	0.00000 0.00000
£91	71 GLU	C	-21.86369 -20.81243	-18.43808	103.51868	Y.)	71 71	0.00000
692 693	71 GLU 72 ILE	о, к	-20.81243 $-22.34609$	-19.31836	104.86364	λl	72	0.00000
694	72 ILE	H	-23,21301	-19.12129	105.33200	ኡነ	72	0.00000
£95	72 ILE	C.R.	-21.56703	-20.53142	105.13649	F. 1	72	0.00000
696	72 ILE	CB	-22.29516	-21.40405	106.17923	1.1	72	0.00000
€97	72 ILE	CG2	-21.51796	-22.68646	105.50604	Al	72 72	0.00000
€9E	72 ILE	CGI	-22.55172	-20.59465 -21.36378	107.43409	23	72	0.00000
€99 700	72 ILE 72 ILE	C C	-23.34520	-21.35378	103.89490	<b>51</b>	72	0.00000
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701	72 ILE		-20. 7	9 -21.68162	103.64178	A1	72	0.00000
702	73 MET		-22.20	6 -21.67127	103.09738	Al	73	0.00000
703	73 MET	н	-23.1780	6 -21.34412	103.27303	λl	73	0.00000
704	73 MET	CA		7 -22.51146			73	0.00000
705	73 MET	CB		7 -23.44601			73	0.00000
706	73 HET	CG		5 -24.44882			73	0.00000
707	73 MET	SD		-25.79652			73 73	0.00000 0.00000
708	73 MET	CE		-26.56731			73	0.00000
709 710	73 MET 73 MET	C		-21.79430 -22.36938		λl	73	0.00000
710	74 THR	о И		2 -20.49214			74	0.0000
712	74 THR	Н		-20.04403			74	0.00000
713	74 THR	Cλ		-19.73833			74	0.00000
714	74 THR	CB		-18.35496			74	0.00000
715	74 THR	OG1		-17.84761		λl	74	0.00000
716	74 THR	HG1	-20.04699	-17.88381	98.02785		74	0.00000
717	74 THR	CG2	-21.20740	-17.31089			74	0.00000
718	74 THR	С		-19.61359			74	0.00000
719	74 THR	0		-19.49348	99.16750		74	0.00000
720	75 LYS	N · · ·		-19.69260			75 75	0.00000 0.00000
721	75 LYS	н		-19.65220			75 75	0.00000
722 723	75 LYS 75 LYS	CA CB		-19.83955 19.57287			75	0.00000
724	75 LYS	CG		-19.66153	103.86107		75	0.00000
725	75 LYS	CD		-19.57437			75	0.00000
726	75 LYS	CE		-19.74395	105.98417		75	0.00000
727	75 LYS	NZ		-19.69891	107.44939		75	0.00000
728	75 LYS	H21		-19.E3508	107.86470		75	0.00000
7.29	75 LYS	HZ2		-18.77551	107.74094		75	0.00000
730	75 LYS	H23		-20.45311	107.77639		75	0.00000
731	75 LYS	C.		-21.21778	101.45102		75 75	0.00000
732 733	75 LYS 76 ARG	o N		-21.36022 -22.25466	100.79660		76	0.00000
734	76 ARG	Н	•	-22.09296	102.44436		76	0.00000
735	76 ARG	CA		-23.61422	101.67525		76	0.00000
736	76 ARG	CB		-24.68494	102.17145		76	0.00000
737	76 ARG	CG		-24.66219	103.62361		76	0.00000
738	76 ARG	CD		-25.98411	103.91795	Al	76	0.00000
739	76 ARG	NE,			105.14334	Al	76	0.00000
740	76 ARG	HE		-25.85364	105.02467		76	0.00000
741	76 ARG	CZ		-26.28686			76	0.00000
742 743	76 ARG 76 ARG	NH1		-26.45770	107.38550		76 76	0.00000
744	76 ARG	HH12		-26.64144 -26.42100	108.30551		76	0.00000
745	76 ARG	NH2		-26.41209	106.51158		76	0.00000
746	76 ARG	HH21		-26.62371	107.39854		76	0.00000
747	76 ARG	нн22			105.72237		76	0.00000
748	76 ARG	С	-17.06072	-23.91761	100.20901	λl	76	0.00000
749	76 ARG	0		-24.45819	99.83552		76	0.00000
750 751	77 SER	ĸ		-23.50462	99.36716		77	0.00000
752	77.SER 77 SER	H CA	-17.80506	-23.05363	99.69917		77 77	0.00000
753	77 SER	CB	-19.13837		97.32351		77	0.00000
754	77 SER	OG	-18.92403		96.24728		77	0.00000
755	77 SER	НG	-18.99574		95.39572		77	0.00000
756	77 SER	С	-17.22854		.97.20137		77	0.00000
757	77 SER	0	-17.39865		96.00106		77	0.00000
758	78 ASN	N	-16.52714		97.97646		78	0.00000
759	78 ASN	H	-16.44843		98.96113		78 78	0.00000 0.00000
760 761	78 ASH 78 ASN	CA CB	-15.74721 -14.33390		97.45264 97.09195		7 E	0.00000
762	78 ASK	CG	-13.52905		98.36114		78	0.00000
763	78 AS:	001	-12.89955		98.89264		78	0.00000
754	78 ASI:	ND2	-13.552(4		98.85326		78	0.00000

./271	_MIN:2.CRI	•	Thu Fab	25 14:58:4	8 1993	13	
765	78 ASN	. una	1 -14.0	2 -23.19170	98.43678 A1	78	0.00000
766	78 ASN		2 -13.0. /			78	0.00000
767	78 ASN			4 -19.72172		78	0.00000
768	78 ASN	ō		8 -19.42979		78	0.00000
769	79 TYR		-17.5961	2 -19.32597		79	0.00000
770	79 TYR		-18.0542	4 -19.55771		79	0.00000
771	79 TYR		-18,2140	8 -18.48918	95.49858 Al	79	0.00000
772	79 TYR	CB	-19.64874	-18.92649	95.21260 Al	79	0.00000
773	79 TYR	CG		5 -20.32764	94.65360 Al	79	0.00000
774	79 TYR	CDI		5 -21.23278	95.25950 ሕጊ	79	0.00000
775	79 TYR	CE1		7 -22.54189	94.75217 Al	79	0.00000
776	79 TYR	CD2		-20.72112	93.54108 Al	79	0.00000
777	79 TYR	CE2		-22.03339	93.03642 Al	79	0.00000
778	79 TYR	CZ		-22.93822	93.64752 A1	79	0.00000
779	79 TYR	ОН		-24.23438	93.18578 A1	79	0.00000
780	79 TYR	нн		-24.30670	92.31232 A1	79	0.00000
781	79 TYR	С		-17.01261	95.83719 A1	79	0.00000
782	79 TYR	0		-16.51273	96.76683 Al	79	0.00000
783 784	80 THR 80 THR	К Н		-16.33235	95.00452 A1	80	0.00000
785	80 THR	CY		-16.79509 -14.92660	94.24288 A1 95.20513 A1	80 80	0.00000
786	80 THR	CB		-14.87711	96.18098 A1	80	0.00000
787	80 THR	061		-13.52440	96,43537 A1	80	0.00000
788	80 THR	HG1		-13.50159	96.80560 A1	80	0.00000
769	80 THR	CG2.		-15.72265	95.72104 A1	80	0.00000
790	BÖ THR	C		-14.32258	93.83840 A1	80	0.00000
791	BO THR	0	-16.16879	-14.97644	92.99811 A1	80	0.00000
792	E1 PRO	R	-17.23243	-13.08096	93.61451 A1	81	0.00000
793	81 PRO	CD		-12.25452	94.50529 Al	81	0.00000
794	81 PRO	CA		-12.43774	92.32255 A1	81	0.00000
795	E1 PRO	ÇВ		-11.39225	92.28996 A1	81	0.00000
796	81 PRO	CG		-10.94901	93.74456 21	81	0.00000
797 798	81 PRO	c		-11.80328	92.25040 A1	81	0.00000
799	81 PRO	ρ.	-15.41926		92.16776 Al	81	0.00000
800	82 ILE	Н И ·	-14.55883 -14.69364		92.27154 Al	82	0.00000
801	82 ILE	СX	-13.18946		92.31920 A1 92.13921 A1	82	0.00000
802	82 ILE	CB	-12.60010		93.53959 A1	€2 82	0.00000
803	82 ILE	CG2	-12.51140		94.38674 Al	82	0.00000
804	82 TE	CG1	-12.31152		93.44331 Al	82	0.00000
805	82 ILE	CD	-10.76554		94.80896 A1	82	0.00000
€06	82 ILE	С	-12.35649		91.37376 A1	82	0.00000
807	82 ILE	OCT1	-11.36717	-12.81747	90.75062 A1	82	0.00000
808	82 ILE	OCT2	-12.72556	-14.37446	91.38671 A1	82	0.00000
809	63 CTA	N	-17.53322	-0.31236	94.99084 Bl	1	0.00000
810	83 GLY	HT1	-17.21994	0.44323	94.35235 B1	1	0.00000
811 612	83 GLY	HT2	-16.86357	-1.12219	94.96444 Bl	1	0.00000
813	83 GTA	HT3 CA	-17.61098	0.01920	95.97150 B1	3	0.00000
814	83 GTA	C	-18.79853 -18.52573		94.55151 B1	1	0.00000
815	83 GLY	ō	-17.35786	-2.38203	94.66351 B1 94.84086 B1	1	0.00000
816	84 ASP	N	-19.57260	÷3.20239	94.59303 B1	2	0.00000
817	84 ASP	H	-20.49658	-2.89510	94.35600 B1	2	0.00000
818	84 ASP	CA	-19.43900	-4.63200	94.86181 B1	2	0.00000
819	84 ASP	CB	-19.44643	-4.83356	96.38475 B1	2	0.00000
820	84 ASP	CG	-18.89301	-6.19619	96.73815 B1	2	0.00000
821	04 ASP	OD1	-17.69451	-6.29764	96.98109 B1	2	0.00000
€22	84 ASP	OD2	-19.66566	-7.14958	96.75715 B1	2	0.00000
823	84 ASP	С	-20.62786	-5.31072	94.19848 Bl	2	0.00000
524 035	84 ASP	0	-21.46903	-4.61697	\$3.63479 B1	2	0.00000
825 826	85 THR 85 THR	N u	-20.67796	-6.64606	94.24891 B1	3	0.00000
827	ES THR	H Ca	-20.04362 -21.75257	-7.15926 -7.39367	94.64032 B1 93.59154 Bi	3 3	0.00000
328	S5 THR	C5	-21.58903	-7.31950	92.05122 B1	3	0.00000 0.00000
			- 2.50903	-1.317-4	VJ122 Bi	-	0.0000

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829	85 THR		-226			3	0,00000
830	85 THR		-22. ,6 -22.7343	5 -7.82480 1 -7.60152		3	0.00000
831	85 THR		-20.3296			3	0.00000
832	85 THR		-21.7429			3	0.00000
833	85 THR		-20.7645			3	0.00000
834	86 ARG	-	-22.8649			4	0.00000
835	86 ARG		-23.6240			4	0.00000
836	86 ARG			-10.87552		4	0.00000
837	86 ARG	CB		-10.79083		4	0.00000
838	86 ARG	CG	-22.74323	-11.65365	96.87092 B1	4	0.00000
839	86 ARG	CD	-23.23116	-13.10294	97.02541 B1	4	0.00000
840	86 ARG	NE		-14.03911	97.27083 Bl	4	0.00000
841	86 ARG	HE		-14.68836	96.53494 Bl	4	0.00000
842	86 ARG	CZ		-14.05016	98.38612 B1	4	0.00000
843	86 ARG	NH1		-14.85617	98.44757 B1	4	0.00000
. 844	86 ARG			-14.87872	99.26299 B1	4	0.00000_
8 < 5	86 ARG			-15.47498	97.69021 81	4	0.00000
846 847	86 ARG 86 ARG	NH2		-13.26636	99.42563 B1	4	0.00000
848	86 ARG				100.26897 B1	4	0.00000
849	86 ARG	C		÷11.82065	99.36831 B1 93.57905 B1	4	0.00000
850	86 ARG	0		-11.52883	93.17882 B1	4	0.00000
851	87 PRO	N		-12.98532	93.27325 B1	\$	0.00000
852	87 PRO	CD		-13.34562	93.54376 B1	5	0.00000
853	67 PRO	C.A.		-14.02757	92.53087 B1	5	0.00000
854	87 PRO	CB		-15.13066	92.39999 B1	5	0.00000
855	62 byo	CG	-21.43460	-14.43376	92.52460 B1	5	0.00000
856	87 PRO	С		~14.54496	93.21975 B1	5	0.00000
857	87 PRO	0		-14.39544	94.41838 E1	5	0.00000
858	88 ARG	N	•	-15.17061	92.39123 B1	6	0.00000
859 860	BB ARG	н		-15.35588	91.44433 B1	6 6	0.00000
861	88 ARG 80 ARG	CA CB		-15.62675 -15.39805	92.90235 B1 91.81653 B1	6	0.00000
862	BB ARG	CG		~15.55859	92.35844 B1	6	0.00000
863	BB ARG	CD		-14.91787	91.49236 B1	6	0.00000
864	BB ARG	NE		-14.57277	92.34607 B1	6	0.00000
8 6 5	88 ARG	HE		-14.64038	93.33788 B1	6	0.00000
866	88 ARG	C2		~14.12165	91.86193 B1	6	0.00000
867	88 ARG	4HJ		-13.81756	92.71322 B1	6	0.00000
£ 68	88 ARG	EH11	-34.95441		92.40144 B1	6	0.00000
869	88 ARG		-33.91853		93.69838 B1	6	0.00000
870 871	88 ARG 88 ARG	NH2		-13.97383	90.54974 B1	6	0.00000
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873	BB ARG	C	-27.23157		93.36366 B1	6	0.00000
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879	89 PHE	CG	-25.20774		95.61829 B1	7	0.00000
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881	89 PHE	CD2	-24.42840		95.96102 B1	7	0.00000
882 883	89 PME	CE1	-23.51045		94.00961 B1	7	0.00000
£84	89 PHE	CE2 CZ	-23.18767 -22.73800		95.32384 B1 94.34976 B1	7	0.00000
285	89 PHE	C	-28.99632		95.72084 B1	7	0.00000
806	89 PHE	ŏ	-29.85551		95.94786 B1	ŕ	0.00000
8 6 7	90 LEU	N		-20.28822	95.87791 B1	ε	0.00000
656	90 LEU	H	-28.38720		95.76376 B1	8	0.00000
883	90 LEU	CA	-30.58975		96.14113 B1	8	0.00000
690	90 LEU	CB	-31.01265		94.64961 B1	8	0.00000
£91	90 LEU	CG	-32.46079		94.43614 B1	8	0.00000
992	90 15U	CDI	-32.8113"	-21.36230	93.19113 21	3	0.0000

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993	90 LEU	CD2		-21.40699	95.55222 B1	8 8	0.00000
894	90 LEU	C	-30.45467	-21.90281	97.20252 B1		0.00000
895	90 LEU	ŏ		-22.89200	97.07224 B1	8	0.00000
	91 TRP	N	-31.28133	-21.71086	98.22982 Bl	9	0.00000
896	91 TRP	H		-20.85226	98.31900 Bl	9	0.00000
897	91 TRP	Ċ.A	-21 61277	-22.86043	99.06700 B1	. 9	0.00000
898	91 TRP	CB	-31.76159	-22.50789	100.54418 Bl	. 9	0.00000
899	91 TRP	CG	_30 46050 ·	-22.11490	101.1813/ 54	-	0.00000
900 901	91 TRP	CD2	-20 22893	-22.79283	101.161/0 51	. 9	0.00000
-	91 TRP	CE2	-28.30074	-21.96546	101.9884/ 54		0.00000
902	91 TRP	CE3	-28.77368	-24 00327	100.60309 02		
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904	91 TRP	NE1	_20 00810	-20.87047	102.44030 B1	. 9	0.00000 0.00000
905	91 TRP	HE1	-28 68566	-20.15616	103.04137 B1	. 9	
906	91 TRP	CZ2	-26 07767	-22.40520	102.165/6 5		0.00000
907	91 TRP		-22 44054	-24.40402	100.81577 B1	. 9	0.00000
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920	92 GLN	HE21	-35.08609	-26.83019	93.40658 B		0.00000
921	92 GLN		-34.37000	-26.35610	99.77327 B	1 10	0.00000
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\$23	92 GLN	٥.	-35.49484	-26.39205		1 11	0.00000
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931	93 LEU	c	->6 93596	-28.11112	101.32695	27 T.T	0.00000
932	93 LEU	ŏ	-37.91692	-27.47571	100.966Z1 E	37 77	0.00000
933	94 LYS	N	-36.95045	-29.41719	101.56549 8	12	0.00000
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941	94 LYS		-42.69798	-34.41995	98.86351		0.00000
942	94 LY6		_42 49249	-33.14263	3 97.78997	81 12	0.00000
943	94 LYS	_	-41 57162	-34.57937	7 97.59540	B1 12	0.00000
944	94 LYS		20 24610	จา กลรจร	1 102.67642	31 12	0.00000
945	94 LYS		_37 54720	-31.99770	102.85849	81 12	0.00000
946	95 PHE	N .	20 40676	-30.8592	, 103.40003	D. 4.5	0.00000
947	95 PHE		20 00321	-30.05201	1 103.34519	RT 73	0.00000
548	95 PHE		20 73794	-31.84982	2 104.4905 <i>3</i> -	81 12	
949	95 PHE		24 12251	-31 49228	A 105.86481 -	F1 13	0.00000
950	95 PHE		20 62106	-30 20B1	9 106.49960	<b>51</b> 13	
951	95 PHE		_20 01617	-28.9668	6 106.12996	בי גם	0.00000
952	95 PHE		40 60668	-30.2647	9 107.511/3	D1 +2	0.00000
953	95 PHE		20 75507	-27 7832	6 106.//YBD	DI 13	0.00000
954	95 PHE	-	45 65/77	29 በጸበነ	5 108.16313	E: 17	0.00000
955	95 PHE		40 /2567		5 10/./9000	5: :-	0.00000
956	95 PHE		-41.22005	-32.1679	9 104.57423	B1 13	0.00000
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95			-42.0. 1 -31.31332 104.41691 B1	13	0.00000
958	3 96 GLt	J N	-41.47812 -33.46734 104.75822 B1	14	0.00000
959	96 GL	JH	-40.74093 -34.09071 105.01948 B1	24	0.00000
960	96 GLt	J CA	-42.80002 -33.99059 104.40078 B1	14	0.00000
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964				14	0.00000
965			The state of the s	14	0.00000
966			-43.13129 -35.25393 105.17925 B1	14	0.00000
967			-42.27510 -36.11395 105.37879 B1	14	0.00000
968	97 CYS		-44.39621 -35.34431 105.62501 B1	15	0.00000
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972	97 CYS	SG	-46.49873 -35.54248 108.42288 B1	25	0.00000 🛴
973	97 CYS	С	-45.89248 -37.36966 105.55706 B1	15	0.00000
974	97 CYS	0	-46.75253 -36.80546 104.88787 B1	15	0.00000
975	98 HIS	N	-45.80356 -38.69951 105.71784 B1	26	0.00000
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986	98 HIS	۵	-47,04279 -40.99638 106.99225 B1	16	0.00000
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988	99 PHZ	H	-49.25243 -39.92869 105.00666 B1	17	0.00000
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999	100 PEE	N	-50.86837 -43.12653 106.85844 B1		0.00000
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020	101 A5%	c	-56.06277 -44.09262 107.83398 B1	19	0.00000

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                         Thu Fab 25 14:58:48 1993
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1086	107	ARG	Ĉ	-42.3	7787	-4	1.03	546	10	6.325	04 Bl	25	
1087		ARG	ŏ	-43.3								25	
1088		LEU	N	-41.3								26	
1089	108	LEU	н	- 40.3								26	
1090	108	Leu	Ċλ	~40.8	9942	-3	9.15	744	10	5.537	51 B1	26	0.00000
1091	108	LEU	CB	-40.8	0087	-3	8.80	954	10	3.012	48 Bl	26	0.00000
1092		LEU	CG	~41.9	6347	-3	7.89	689	108	3.358	74 B1	26	0.00000
1093			CD1	-42.7								26	0.00000
1094			CDS	-41.5								26	0.00000
1095			C	-39.6								26	0.00000
1096	108 109		0	-38.7								26 27	0.00000 0.00000
1098	109		N H	-39.5 -40.2								27	0,00000
1099	109		Cλ	-38.3								27	0.00000
1100	109		CB	-38.4								27	0.00000-
1101	109		CG	-39.7								27	0.00000
1102	109		CD1	-39.4								27	0.00000
1103	109	LEU	CD2	-40.4								27	0.00000
1104	109	LEU	c·•	-37.9								27	0.00000
1105	109		0	-38.81								27	0.00000
1106	110		N	-36.70								28	0.00000
2107	110.0		11	-36.03								28	0.00000
1108	110 (		CΣ	~36.20								28	0.00000
1110	110 (		CB	-35.80 -35.32								28 28	0.00000
1111	110		CD	-33.83								28	0.00000
1112	110		OE1	-33.37								28	0.00000
1113	110		OE2	-33.09								28	. 0.00000
1114		grų	C	-35.01	026	-33	.940	76	104	.1550	0 Bl	28	0.00000
1115	110 6	SLU	0	-34.25	577	-34	.908	07		.1158		28	0.00000
1116	222 2		N	-34.85	(39	-32	.868	43	103	.3722	2 B1	29	0.00000
1117	111 /		H	-35.61								29	0.00000
1118	111 /		CA	-33.75								29	0.00000
1119	111 /		CB	-33.99						.2035		29	0.00000
1121	111 7	ARG	CG CD	-35.45 -35.67						.7530 .7517		29 29	0.00000
1122	111 2		NE	-37.09						.7261		29	0.00000
1123		<b>IRG</b>	HE	-37.71						.2275		29	0.00000
1124	111 Å		CZ	-37.50						.0978		29	0.00000
1125	111 A		NHI	-38.78	116	-36	. 6891	71	99	1611	9 Bl	29	0.00000
1126		LRG		-39,12					98.	6827	6 Bl	29	0.00000
1127		JRG		-39.43						7094		29.	0.00000
1128 1129			NH2	-36.63						4151		29	0.00000
1130		JRG JRG	nnaa	-36.91	201	-37	. 9034	8		9432.		29	0.00000
1131			C	-35.67 -33.49	125 .	~J6.	. /000			3626		29	0.00000
1132			ŏ	-34.39						2660		29 29	0.00000
1133	112 C		ĸ	-32.20								30	0.00000
1134	112 C		H.	~31.50								30	0.00000
1135		YŞ	CA	-31.80	458 -	-29.	6236	0 1	101.	7382	5 Bl	30	0.00000
1136	112 C		CB	-31.12								30	0.00000
1137 1138	112 C		5G	~30.70								30	0.00000
1139	112 C			-30.87								30	0.00000
1140	113 1			-29.97; -31.15						65078		30	0.00000
1141				-31.15: -31.84:						86111		31 31	0.00000 0.00000
1142				-30.55						32464		31	0.00000
1143				-31.560						30704		31	0.00000
1144		LE ·		-33.00						82323		31	0.00000
1145				-31.52						69635		31	0.00000
1146 1147				-32.440						93272		31	0.00000
1148				-30.08						96536		31	0.00000
	113 1	LE	0	~30.75	::3 -	· 2 % .	2590	U	76.	21317	81	31	0.00000

	15	ಚಿ.ರಾ೨		Thu Fab	25	14:	58:	48 1	993			19	
. ,	21	TYR	N	-28. /1	0 -:	27.2	:556	4 9	7.4	1665	81	32	0.00000
<b>1150</b>		TYR	H	-28.4297				9		0297		32	0.00000
1151		TYR	CA	-28.2203						1462		32	0.00000
1152	114	TYR	CB	-26.8008						1345		32 32	0.00000
1153		TYR	සා	-26.0112° -26.6277						1311 9068		32	0.00000
1155		TYR	CEI	-25.8488						5267		32	0.00000
1156		TYR	CD2	-24.6182						8751		32	0.00000
1157		TYR	CE2	-23.8384					7.3	4588	Bl	32	0.00000
1158		TYR	CZ	-24.45600			-			3154		32	0.00000
1159		TYR	OH	-23.6896				-		979		32	0.00000
1160 1161		TYR TYR	нн	-22.79676 -28.14723				-		1984 1430		32 32	0.00000
1162	114		C	-27.66375						236		32	0.00000
1163		ASN	N	-28.66823						919		33	0.00000
1164		ASN	H	-29.03092					5.77	643	Bl	33	0.0000
1165	115		CA	-28.63762	-2	4.4	1545	9:	3 . 66	566	Bl	33	0.00000
1166		ASN	CB	-27.27049						078		33	0.00000
1167		ASN	CG	-27.00239						1440		33	0.00000
1168 1169		ASN	ND2	26.55389−27.51765 27.51765−						271		33 33	0.00000
1170		ASN		-28.04883						797		33	0.00000
1171		ASN	HD22	-27.29583						946		33	0.00000
1172		ASN	С	-28.96318						321		33	0.00000
2173		ASN	0	-28.22150	-2	5.9	1402			250		33	0.00000
1174		GLN	N	-30.10691						767		34	0.00000
1175		GLN	H Cr	-30.66790						830		34	0.00000
1176 2177	116	GLN	CA CB	-30.60575 -30.73906						212 631		34 34	0.00000
1178		GLN	CG.	-31.33401						983		34	0.00000
1179	116		CD	-31.33954						588		34	0.00000
1180	116		OE1	-32.32002						605		34	0.00000
1181	116		NE2	-30.20428						185		34	0.00000
1182 1183	116		HE21 HE22	-29.39553						205		34 34	0.00000 0.00000
1184	116		C.	-30,15594 -29,89899						205 043		34	0.00000
1185	116		ο.	-30.38571						767		34	0.00000
1186	117	GLU	N	-28.76921						838		35	0.00000
1187	1j2	CTA	H	-28.34990				93	. 59	525	Bl	35	0.00000
1188	117	GLU	CA	-28.17324						636		35	0.0000
1189	117	GLU	CB	-26,68237						572		35	0.00000
1190 1191	117	GLŲ GLŲ	CD	-26.41125 -24.93459						724		35 35	0.00000
1192	117	GLU .	OE1	-24.62388						636 359		35	0.00000 0.00000
1193	117	GLŲ	OE2	-24.09945						135		35	0.00000
1194		GLU	С.	-28.34342	-30	3.39	133			360		35	0.00000
1195 1196		GLU	0 .	-28.39032						593		35	0.00000
1197		GLU	N H	-28.45418 -28.37884					•	151		36	0.00000
1198		GLU	CA	-28.64640			663 718			856 504		36 36	0.00000
1199		GLU	CB	-28.86529						220		36	0.00000
	118		CG	-30.04621	-34	. 25	904	96	.04	454	B1	36	0.00000
1201	118		CD	-30.18685				96	. 39	969	Bl	36	0.00000
1202	118			-31.31366						004		36	0.00000
1203 2204	118 118		OE2 C·	-29.17775 -27.45968						236 954		36 36	0.00000
	118			-26.30375						955 004		36 36	0.00000
	119			-27.77719						671		37	0.00000
1207	119		H	-28.73032	-31	22	468			568		37	0.00000
3022	119			-26.67523						333		37	0.00000
	119			-26.79679								37	0.00000
	119 119			-25.62406 -25.73940								37 37	0.00000 0.00000
	115			-26.64967								37	0.00000

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1213	3 11	9 SE	٥ ه	-25.74	.8 -3	2.9055	4 10	1 03211	R1	37	0.00000
1214		O VAI	, N	-27.7243	4 -3	2.0680	8 10	1.67562	81	38	0.00000
1215		O VAI		-28.5002	26 -3	1.4593	8 10	1.48344	B1	38	0.00000
1216	12	O VAI	CA	-27.8267	B -3	2,9980	2 10	2.80099	B1	38	0.00000
1217		0 VA1		27.4479	0 -3	2.3224	4 10	4.13868	Bl	38	0.00000
1218		O VAI		-25.9325						38	0.00000
1219		0 VAI	_	-28.1563						38	0.00000
1220		O VAL	_	-29.2377						38	0.00000
1221		0 VAL 1 ARG		-30.1981						38	0.00000
1223		1 ARG	-	-29.3416 -28.5252						39	0.00000
1224		1 ARG		-30.6594	-					39 39	0.00000
1225	12:	ARG	CB	-30.8387						39	0.00000
1226		LARG	CG	-32.2489						39	0.00000
1227		ARG	CD	-32.3644						39	0.00000
1228		ARG	NE	-33.4663						39	0.00000-
1229		ARG	HE	-33.5831						39	0.00000
1230	121	ARG	CZ	-34.2177						39	0.00000
1231		ARG	NH1	-35.1884						39	0.00000
1232		·ARG		-35.7797						39	0.00000
1233		ARG		-35.3336						39	0.00000
1234 1235		ARG	NH2	-33.9978				.82444		39	0.00000
1236		ARG		-34.53079 -33.27054				.25675		39 39	0.00000
1237		ARG	C	-30.80743						39	0.00000
1238		ARG	ŏ	-29.86515						39	0.00000
1239		PHE	N	-32.04075						40	0.00000
1240	122		H	-32.75061						40	0.00000
1241		PHE	CA	-32.40666						40	0.00000
1242	122		CB	-33.75724	-36	.87165	106	.85296	Bl	40	0.00000
1243		SHE	CG	-33.64992	-36	.45831	108	.30418	Bl	40	0.00000
1244		PHE	CD1	-32.56100	-35	.69712	108	.77664	BI	40	0.00000
1245		PHE	CD2	-34.66985						€0	0.00000
1246		PHE PHE	CE1	-32.49275						40	0.00000
1248		PHĖ	CE2 Cz	-34,60187 -33.51285						40	0.00000
1249	122		c	-32.57844	-39	. 13023 . 52121	105	60697	21 21	40 40	0.00000
1250	122		ō	-33.34168	-38	.7920B	104	65587	B)	40	0.00000
1251		ASP	N	-31.86201	-39	. 60796	106.	15389	Bl	41	0.00000
1252		ASP	н	-31.23184	-39.	47015	106.	92548	B1	41	0.00000
1253 1254		ASP	CA	-32.08552	-40.	. 93522	105.	58825	Bl	41	0.00000
1255	123	ASP	CB	-30.85171	-41	. B1726	105.	76445	B1	41	0.00000
1256	123		CG OD1	-29.93161 -28.81173	-41.	.56041	104.	59405	B1	41	0.00000
1257		ASP		-30.34905	-41	11310	109.	45856	B1	41 41	0.00000
1258	123		С	-33.32362	-41	63618	106	09965	B)	41	0.00000
1259	123	ASP	0	-34.00966	-41.	21121	107.	02319	B1	41	0.00000
1260		SER	н	-33.62443	-42.	74250	105.	41429	B1	42	0.00000
1261		SER	H	-32.95329	-43.	10971	104.	76900	B1	42	0.00000
1262 1263		SER,		-34.94425						42	0.00000
1264	124	SER	CB	-35,18779	-44.	37028	104.	46149	B1	42	0.00000
	124			-36.57945						42	0.00000
1266	124	SER		-36.91089 -35.21640	-44.	01057	105.	4/913   07624	p t p T	42 42	0.00000
1267	124			-36.33538						42	0.00000
1268	125	ASP	и .	-34.16447	-44.	10325	107.	74330	B1	43	0.00000 0.00000
1269	125	ASP	H ·	-33.26228	-43.	73425	107.	50494	B1	43	0.00000
	125		CA -	-34.30492	-44.	60689	109.	10471 :	31	43	0.00000
	125			-32.96210						43	0.00000
	125			-31.82155		_				43	0.00000
	125 125	¥25		-31.89194						43	0.00000
	125			-30.87249						43	0.00000
	125			-34.69374 -35.10540						43 43	0.00000
	,		_	-3.16340	. 45.	. 5 4 4 4			- 1	٦,٥	0.00000

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1277	126 VA	. ห	-34.51	-42.26751	109.64790 B	44	0.00000
1278	126 VA				108.70456 B	. 44	0.00000
1279	126 VA1				110.50496 B		0.00000
1280	126 VAI				110.97592 B		0.00000 0.00000
1281	126 VAI 126 VAI				111.54094 B1 109.82481 B1		0.00000
1282 1283	126 VAI				111.64961 B		0.00000
1284	126 VAI				112.79533 B1		0.00000
1285	127 GLY				111.25324 B3		0.00000
1286	127 GLY	. H	-32.31598	-42.01122	110.31755 BI	. 45	0.00000
1287	127 GLY				112.19529 B1		0.00000
1288	127 GLY				111.62542 B1		0.00000
1289	127 GLY	-	-29.03055 -29.03055	-41.21776	112.35962 B1 110.29545 B1		0.00000
1290 1291	128 GLU				109.72534 B1	46	0.00000
1292	128 GLU			-41.14297		46	0.000007_
1293	128 GLU				109.11709 B1	46	0.00000
1294	128 GLU				109.59860 B1	46	0.00000
1295	128 GLU			-43.28422		46 46	0.00000 0.00000
1296 1297	128 GLU	OE2			108.19992 B1 109.00348 B1	46	0.00000
1290	128 GLU	C			108.75031 B1	46	0.00000
1299	128 SLU	ō			108.35724 B1	46	0.00000
1300	129 TYR	N		-39.42619		47	0.00000
1301	129 TYR	н	-25.68498	-39.83420	108.68820 B1	47	0.00000
2302	129 TYŔ			-38.29454		47	0.00000
1303	129 TYR	E3		-37.15326		47	0.00000
1304	129 TYR 129 TYR	CG CD1		-36.34222 -36.21958	109.09443 B1 110.34811 B1	47 47	0.00000
1305	129 TYR 129 TYR	CE1		-35.42131			0.00000
1307	129 TYR	CD2		-35.67832		47	0.00000
2308	129 TYR	CE2		-34.88063		47	0.00000
1309	129 TYR	CZ		-34.75726		47	0.00000
1310	129 TYR	OH		-33.98459		47	0.00000
1311 1312	129 TYR 129 TYR	нн			111.67732 B1 106.15941 B1	47 47	0.00000
1313	129 TYR	CO		-39.04407		47	0.00000
1314	130 ARG	ĸ		-38.38162	105.08581 B1	48	0.00000
1315	130 ARG	н		-38.10451	105.16735 B1	48	0.00000
1316	130 ARG	CA	•	-38.41254	103.80227 B1	48	0.00000
1317 1318	130 ARG	CB		-38.84699	102.71647 B1	48	0.00000
1319	130 ARG 130 ARG	CG		-39.00526	101.34112 B1	48	0.00000
1320	130 ARG	'NE		-39.41974 -39.38333	100.29808 B1 98.95629 B1	48 48	0.00000
2321	130 ARG	HE		-38.85034	98.82833 Bl	48	0.00000
1322	130 ARG	CZ		-39.96348	.97.93202 Bl	48	0.00000
1323	130 ARG	KHI		-39.81313	96.69917 B1	48	0.00000
1324 1325	130 ARG 130 ARG		-28.26738		,95.90996 Bl	48	0.00000
1326	130 ARG 130 ARG	NH2	-27.01064	-40.68730	96.53955 B1 98.14392 B1	48 48	0.00000 0.00000
1327	130 ARG		-29.90446		97.39118 B1	48	0.00000
1328	130 ARG		-29.72741		99.07957 Bl	48	0.00000
1329	130 ARG	C	-26.28084	-37.06053	103.45986 Bl	48	0.00000
1330	130 ARG	0			103.07688 B1	48	0.00000
1331 1332	131 ALA	N			103.58668 Bl	49	0.00000
1333	131 ALA 131 ALA	H CA			103.95192 B1 102.98902 B1	49 49	0.00000
1334	131 ALA	CB			103.80801 B1	49	0.00000
1335	131 ALA	Č			101.58658 B1	49	0.00000
1336	131 ALA	0	-23,17892	-37.20532	101.36065 B1	49	0.00000
1337	132 VAL	N			100.63154 B1	50	0.00000
1338 1339	132 VAL 132 VAL	li Or	-24.78984		100.25567 Bl 99.24192 Bl	50 50	0.00000 0.00000
1340	132 VAL	CA CB		-35.11200	98.36560 B1	50 50	0.00000
				20			

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	120		25 ^	5 -3E 45 CO		50	0.00000
1341 1342				5 -35.4568° 8 -35.4889			0.00000
1343				6 -35.5339			0.00000
1344				8 -36.1925			0.00000
1345				6 -34.5356			0.00000
1346					2 100.11190 B1		0.00000
1347				7 -34.13851			0.00000
134B				9 -33.09962			0.00000
1349	_			9 -32.56708			0.00000
1350	133 TH	R HG1	-19,6901	8 -32.10136	96.50551 B1	51	0.00000
1351	133 TH	R CG2	-21.8173	0 -31.96947	98.12788 B1	51	0.00000
1352	133 TH	R C			100.10846 B1	51	0.00000
1353	133 TH				101.15881 B1	51	0.00000
1354	134 GL			9 -33.44216		52	0.00000
1355	134 GLT			2 -33.65725		52	0.00000
1356	134 GLI				100.97647 B1	52	0.00000
1357	134 GLU				100.49482 B1	52	0.00000
1358	134 GLU				100.03844 B1	52	0.00000
1359 1360	134 GLU			-34.04410		52	0.00000
1361	134-GLU 134 GLU				99.88007 B1	52 52	0.00000
1362	134 GLU			33.03519 -31.51310	98.99487 B1 101.45728 B1	52	0.00000
1363	134 GLU				102.59352 B1	52	0.00000
1364	135 LEU				100.55812 B1	53	0.00000
1365	135 LEU			-31.13340		53	0.00000
1366	135 LEU				100.94931 B1	53	0.00000
1367	135 LEU	CB		-29.06218		53	0.00000
1368	135 LEU	CG		-27.57937		53	0.00000
1369	135 LEU				100.32666 B1	53	0.00000
1370	135 LEU			-27.23870	,99.36436 B1	53	0.00000
1371	135 LEU			•	102.11412 B1	53	0.00000
1372 1373	135 LEU			-28.93514		53	0.00000
1374	136 GLY				102.02891 B1 101.30480 B1	54 54	0.00000
1375	136 GLY		•		101.30430 B1	54	0.00000
1376	136 GLY	C			104.26834 B1	54	0.00000
1377	136 GLY				105.38053 B1	54	0.00000
1378	137 ARG	N			104.01306 B1	55	0.00000
1379	137 ARG	Ħ	-20,17033	~32.57514	103.08296 B1	55	0.00000
1380	137 ARG	CA	-19.94165	~33.32437	105.09532 B1	55	0.00000
1381	137 ARG	CB			104.58318 B1	55	0.00000
1382	137 ARG	CG			105.55025 B1	55	0.00000
1383 1384	137 ARG	CD			105.85371 B1	55	0.00000
1385	137 ARG 137 ARG	NE.			106.87657 Bl	S5	0.00000
1386	137 ARG 137 ARG	HE Cz			107.47204 B1 107.07086 B1	55	0.00000
1387	137 ARG	NH1			107.07686 B1	55 55	0.00000
1388	137 ARG				108.14749 B1	55	0.00000 0.00000
1389	137 ARG	HH12	~17.88763	-38.75541	108.49972 B1	55	0.00000
1390	137 ARG	NH2			106.37214 B1	55	0.00000
1391	137 ARG				106.49834 B1	55	0.00000
1352	אָאָ רצו				105.70437 B1	55	0.00000
1393 1394	137 ARG		-19.76338	-32.65026	106.46929 B1	55	0.00000
1395	137 ARG 138 PRO	0	-20.33202	-33.13638	107.44172 B1	55	0.00000
1395	138 PRO	N CD	-18 25002 -18 25002	-31.31331	106.56277 B1 105.55482 B1	56 56	0.00000
1357	138 PRO	CA			107.87839 B1	56 56	0.00000
1398	138 PRO	CB			107.61418 B1	56	0.00000
1399	138 PRO	CG			106.35369 B1	56	0.00000
1400	136 PRO	c			108.45452 B1	56	0.00000
1401	136 PRO	o	-20.38873	-30.20105	109.65243 B1	56	0.00000
1402	139 ASP	71			107.56513 B1	57	0.00000
1403	139 352	H			106.60295 21	57	0.00000
1404	139 AST	CA	-22.54445	-29.76374	108.02635 B1	57	0.00000

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1405	139 ASP	СВ		-29,22794			57	0.00000
1406	139 ASP	CG		-28.44150			57	0.00000
1407	139 ASP	OD1		-27.25955			57	0.00000
1408	139 ASP	OD2		-29.00937			57	0.00000
1409	139 ASP	С		-30.90651			57	0.00000
1410	139 ASP	0		-30.79944			57	0.00000
1411	140 ALA	N	-23.18867	-32.06950	108.04975	Bl	5 B	0.00000
1412	140 ALA	H	-22.77745	-32.09325	107.13514	Bl	58	0.00000
1413	140 ALA	CA	-23.64141	-33.29863	108.70194	<b>B</b> 1	58	0.00000
1414	140 ALA	CB	-23.39932	-34.51285	107.80148	B1	58	0.00000
1415	140 ALA	С	-22.96994	-33.52591	110.04660	Bl	58	0.00000
1416	140 ALA	0	-23.61501	-33.62460	111.08086	Bl	58	0.00000
1417	141 GLU	N	-21.63141	-33.53710	110.01537	В1	59	0.00000
1418	141 GLU	H	-21.14260	-33.44422	109.14251	Bl	59	0.00000
1419	141 GLU	CA	-20.88131	-33.73045	111.26272	Bl	59	0.00000
1420	141 GLU	CB	-19.38545	-33.75474	110.92637	<b>B</b> 1	59	0.00009
1421	141 GLU	CG		-34.92155			59	0.00000-
1422	141 GLU	CD	-17.65605	-34.91070	109.44677	Bl	59	0.00000
1423	141 GLU	OE1	-17.21662	-35.95752	108.96182	Bl	59	0.0000
1424	141-GLU	· OE2	-16.99658				59	0.00000
1425	141 GLU	С		-32.72395			59	0.00000
1426	141 GLU	0		-33.05368			59	0.00000
1427	142 TYR	N		-31.47026			60	0.00000
1428	142 TYR	H		-31.22939			60	0.00000
1429	142 TYR	CA	-21.91640	-30.42572	112.62625	Bl	60	0.00000
1430	142 TYR	CB	-22.17510	-29.18770	111.95478	Bl	60	0.00000
1431	142 TYR	CG		-27.86866			60	0.00000
1432	142 TYR	CD1		-27.21121			60	0.00000
1433	142 TYR	CEl		-25.94177			60	0.00000
1434	142 TYR	CD5		-27.27306			€0	0.00000 0.00000
1435	142 TYR	CE2		-26.00211			60	0.00000
1436	142 TYR	CZ		-25.34007			60	0.00000
1437	142 TYR	ОН		-24.08718			60	0.00000
1438	142 TYR	нн		-23.75980				0.00000
1439	142 TYR	C		-30.84932			60	0.00000
1440	142 TYR	0		-30.86335			60 61	0.00000
1441	143 TRR	11		-31.24530	111.69669		6 <u>1</u>	0.00000
1442 1443	143 TRP	H.		-31.27353 -31.65772			61	0.00000
1444	143 TRP	CA CB		-31.82534	112.10045		61	0.00000
1445	143 TRP	CG		-30.51319			61	0.00000
1445	143 TRP	CD2		-30.35383			61	0.00000
1447	143 TRP	CE2		-28.88192			61	0.00000
1448	143 TRP.	CE3		-31.24445			61	0.00000
1449	143 TRP	CD1		-29.20408			61	0.00000
1450	143 TRP	NEI		-28.24161			61	0.00000
1451	143 TRP	HE1	-26.86335	-27.27405	111.09738	B1	61	0.00000
1452	143 TRP	CZ2	-28.41151	-28.41903	108.90296	Bl	61	0.00000
1453	143 TRP	C23	-28.94655	-30.73482	108.27096	B1	61	0.00000
1454	143 TRP.	CH2	-29.03488	-29.34388	108.03833	Bl	61	0.00000
1455	143 TRP	C·	-25.40824	-32.93379	114.07770	Bl	61	0.00000
1456	143 TRP	Ο.		-33.11650			61	0.00000
1457	144 ABN	N		-33.80055			62	0.00000
1458	144 ASN	H		-33.62305			62	0.00000
1459	144 ASN	CA		-34.99080			62	0.00000
1450	144 ASN	CB	-23.20850	-35.93308	113.73882	B1	62	0.00000
1461	144 ASK	CG	-23.89541	-36.68861	112.61740	21	62	0.00000
1462	144 ASN	ODl		-36.47075			62	0.00000
1463	144 ASN	ND2		-37.64097			62	0.00000 0.00000
1464 1465	144 ASN		-24.69338				62 62	6.00000
1465	144 ASN 144 ASN		-25.19584	-38.20406	114 97501	B1	62	0.00000
1467	144 ASN	0	-23.490/3	-35.54654	116.69934	B1	62	0.00000
1461	145 SER	1;	-22.43003	-33.346640	115 07353	31	€3	0.00000
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1469	145 SE			10 -30 -044			0.00000
1470			-22.'	10 -32.8042	28 115.21961 B1 21 117.25865 B1	63 63	
1471					54 117.25065 B1	63	
1472					0 118.24511 B1	63	0.00000
1473					5 118.91065 B1	63	0.00000
1474					4 118.06161 B1	63	0.00000
1475	145 SER	-			7 119.13941 B1	63	0.00000
1476	146 GLN				7 117.51252 B1	64	0.00000
1477	146 GLN				4 116.64774 B1	64	0.00000
1478	146 GLN				6 118.19522 B1	64	0.00000
1479	146 GLN	CB			1 117.23892 B1	64	0.00000
1480	146 GLN	CG			5 117.72882 B1	64	0.00000
1481	146 GLN	CD			2 117.25234 B1	64	0.00000
1482	146 GLN	OE1	-27.8083	7 -27.5360	9 118.00911 B1	64	0.00000
1463	146 GLN	NE2	-27.0655	6 -27.9794	8 115.94329 B1	64	0.00000
1484	146 GLN	HE21	-26.3080	9 -28.2034	9 115.33276 Bl	64	0.00000
1485	146 GLN	HE22			7 115.56134 B1	64	0.00000
1486	146 GLN	C			4 118.57642 B1	64	0.00000
1487	146 GLN	0			9 117.77294 B1	64	0.00000
1488	147 -LYS				6-119-82371 B1	65	0.00000
1489 1490	147 LYS 147 LYS	H			9 120.47663 B1	65	0.00000
1491	147 LYS	CA			4 120.21964 Bl	65	0.00000
1492	147 LYS	CB			1 121.37895 B1 6 121.84203 B1	65 65	0.00000
1493	147 LYS	CD			2 121.97244 B1	(5	0.00000
1494	147 LYS	CE			5 121.47444 B1	65	0.00000
1495	147 LYS	NZ			4 121.26907 B1	65	0.00000
1496	147 LYS	HZ1			3 120.71767 B1	65	0.00000
1497	147 LYS	HZ2			120.68922 B1	65	0.00000
1498	147 LYS	HZ3			2 122.15073 B1	65	0.00000
1499	147 LYS	C			9 119.09340 B1	65	0.00000
1500	147 LYS	٥	-29.3023	5 -32.90174	118.83883 B1	65	0.00000
1501	148 ASP	N	-27.34620	7 -34.00916	5 118.45822 B1	66	0.00000
1502	148 ASP	H			118.75300 B1	66	0.00000
1503	148 ASP	CA			117.48362 B1	66	0.00000
1504 1505	148 ASP	CB	-27.88927	7 -36.37833	118.17059 B1	66	0.00000
1506	148 ASR 148 ASP	CG	-26.79528	-36.57930	119.21505 B1	66	0.00000
1507	148 ASP	OD1 OD2			119.05193 B1 120.23524 B1	66 66	0.00000
1508	148 ASP	_			116.79645 B1	€6	0.00000
1509	148 ASP	ŏ .			117.04951 B1	€6	0.00000
1510	149 LEU	N			115.93941 B1	67	0.00000
1511	149 LEU	H			115,73440 B1	67	0.00000
1512	149 LEU	CA			115.45008 B1	67	0.00000
1513	149 LEU	CB			114.57360 B1	67	0.00000
1514	149 LEU	CG			114.02475 B1	67	0.00000
1515	149 LEU	CD1			112.65290 B1	67	0.00000
1516	149 LEU	CD2			115.02072 B1	67	0.00000
1517 1518	149 LEU	Ç			114.80952 B1	67	0.00000
1519	149 LEU 150 LEU	0			114.83807 B1	67	0.00000
1520	150 LEU	H Ņ			114.32363 B1	68	0.00000
1521	150 LSU		-23,733/3	-34.94139	114.11621 B1 114.12850 B1	68 68	0.00000
1522	150 LEU	CB			114.12830 B1 114.15286 B1	68	0.00000
1523	150 LEU	CG			114.15266 B1 112.89569 B1	68	0.00000
1524	150 LEU	CD1			113.18796 B1	68	0.00000
1525	150 LEU	CD2			121.73915 B1	65	0.00000
1526	150 LEU	С			115.10785 B1	65	0.00000
1527	150 LEU	Ö			114.70350 B1	63	0.00000
1528	151 GLU	N	-32.47441	-36.43576	116.39428 B1	69	0.00000
1529	151 GLU	H			116.72119 B1	69	0.00000
1530	151 GLU	CA			117.30950 B1	6.9	0.00000
1531	151 GLU	CB			118.72928 B1	69	0.00000
1532	151 GTA	CG	-32.69081	-35.41906	118.86324 Pl	62	0.00000

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1533 151 GLU CD -31.15.67 -38.44464 118.70497 E1 69 0.00000 1534 151 GLU OC2 -30.51522 -38.56462 119.72459 B1 69 0.00000 1536 151 GLU OC2 -30.51522 -38.56462 119.72459 B1 69 0.00000 1536 151 GLU O -35.75790 -35.73131 17.56467 B1 69 0.00000 1538 152 GLN N -33.98601 -34.19700 117.35586 B1 70 0.00000 1538 152 GLN N -33.98601 -34.19700 117.35586 B1 70 0.00000 1538 152 GLN CA -34.69656 -33.04752 117.40695 B1 70 0.00000 1540 152 GLN CA -34.69656 -33.04752 117.40695 B1 70 0.00000 1541 152 GLN CB -34.15680 -31.71646 117.32018 B1 70 0.00000 1541 152 GLN CB -34.15680 -31.71646 117.32018 B1 70 0.00000 1541 152 GLN CB -33.23376 -29.77424 118.49381 B1 70 0.00000 1541 152 GLN CB -33.23376 -29.77424 118.49381 B1 70 0.00000 1541 152 GLN CB -33.23376 -29.77424 118.49381 B1 70 0.00000 1545 152 GLN MEZ -34.3656 -29.04662 118.54711 B1 70 0.00000 1546 152 GLN MEZ -34.3656 -29.04662 118.54711 B1 70 0.00000 1546 152 GLN MEZ -34.3656 -29.04662 118.54711 B1 70 0.00000 1546 152 GLN MEZ -34.26188 -28.05358 118.46911 B1 70 0.00000 1546 152 GLN MEZ -34.26188 -28.05358 118.46911 B1 70 0.00000 1546 152 GLN MEZ -34.26188 -28.05358 118.46911 B1 70 0.00000 1549 152 GLN O -35.89575 -33.04746 116.27182 B1 70 0.00000 1550 153 ANG N -35.34435 -33.30759 115.08552 B1 71 0.00000 1550 153 ANG N -35.34435 -33.30759 115.08552 B1 71 0.00000 1555 153 ANG C -36.25853 -33.34709 114.99299 B1 71 0.00000 1555 153 ANG C -36.25853 -33.34709 114.99299 B1 71 0.00000 1554 153 ANG C -34.84260 -32.07791 112.35564 B1 71 0.00000 1556 153 ANG N -34.35839 -33.46709 114.99299 B1 71 0.00000 1556 153 ANG N -34.35839 -33.46709 114.99299 B1 71 0.00000 1556 153 ANG C -34.84260 -32.07791 112.35564 B1 71 0.00000 1556 153 ANG C -36.28635 -33.0219 112.35564 B1 71 0.00000 1556 153 ANG C -36.28635 -33.0219 112.35564 B1 71 0.00000 1556 153 ANG N -32.35317 -30.95360 110.55166 B1 71 0.00000 1556 153 ANG C -37.5655 -38.3849 -32.25700 111.7839 B1 71 0.00000 1556 153 ANG C -37.5655 -38.3849 -39.22906 100.55480 B1 71 0.00000 1556 153 ANG C -37.5655 -30.00000 10.5586 B1 71 0.00000 1556 153 A	. / שעו	_KINY.CRD	ı	בשמ ד ר	25 14:58:	48 1993	25	
1535 151 GLU OE2 -30.51522 -38.56462 119.72459 81 69 0.00000 1537 151 GLU O -34.55067 -35.41168 117.48557 81 69 0.00000 1538 152 GLN N -33.98601 -34.19700 117.550647 81 69 0.00000 1539 152 GLN N -33.98601 -34.19700 117.550687 81 70 0.00000 1540 152 GLN CA -34.68656 -33.04752 117.18607 81 70 0.00000 1541 152 GLN CB -34.15600 -31.71646 117.32018 81 70 0.00000 1541 152 GLN CB -34.15600 -31.71646 117.32018 81 70 0.00000 1542 152 GLN CB -34.15600 -31.71646 117.32018 81 70 0.00000 1543 152 GLN CB -33.23376 -29.77424 118.49387 81 70 0.00000 1544 152 GLN CB -33.23376 -29.77424 118.49387 81 70 0.00000 1544 152 GLN OE1 -32.13068 -29.27019 118.36008 81 70 0.00000 1544 152 GLN NEJ -34.35656 -29.04652 118.54711 81 70 0.00000 1545 152 GLN NEJ -34.213068 -29.47511 118.65663 81 70 0.00000 1547 152 GLN NEZ -34.28168 -28.0555 81 118.46911 81 70 0.00000 1549 152 GLN C -35.89575 -33.04746 116.27182 81 70 0.00000 1549 152 GLN C -35.89575 -33.04746 116.27182 81 70 0.00000 1549 152 GLN C -35.89575 -33.04746 116.27182 81 70 0.00000 1549 152 GLN C -35.89575 -33.04746 116.27182 81 70 0.00000 1552 153 ANG N -35.34453 -33.8539 115.08552 81 71 0.00000 1552 153 ANG N -35.34453 -33.8539 115.08552 81 71 0.00000 1552 153 ANG C -36.28553 -33.42191 119.59547 81 71 0.00000 1554 153 ANG C -34.84260 -32.07791 112.35548 81 71 0.00000 1554 153 ANG C -34.84260 -32.07791 112.35548 81 71 0.00000 1555 153 ANG C -34.84260 -32.07791 112.35548 81 71 0.00000 1555 153 ANG C -34.84260 -32.07791 112.35548 81 71 0.00000 1555 153 ANG C -34.84260 -32.07791 112.35548 81 71 0.00000 1556 153 ANG C -33.88599 -32.22570 111.17839 81 71 0.00000 1556 153 ANG C -33.88599 -32.22570 111.17839 81 71 0.00000 1556 153 ANG C -34.84260 -32.07791 112.35548 81 71 0.00000 1556 153 ANG C -34.84260 -32.07791 112.35548 81 71 0.00000 1556 153 ANG C -34.84260 -32.07991 112.35548 81 71 0.00000 1556 153 ANG C -34.84260 -32.07991 112.35548 81 71 0.00000 1556 153 ANG C -34.84260 -32.07991 112.35548 81 71 0.00000 1556 153 ANG C -34.84260 -32.07991 112.35548 81 71 0.00000 1556 153 ANG C -33.85	. 2533	151 GLU	CD	-31.15_8	7 -38.4446	4 118.70497 E1	69	0.00000
1536   151   GLU   C   -34.55067 -35.41168   137.4885   B1   69   0.00000     1538   152   GLN   N   -33.98601 -34.19700   117.35566   B1   70   0.00000     1539   152   GLN   K   -33.00321 -34.10256   17.18602   B1   70   0.00000     1540   152   GLN   C   -34.89656 -33.04752   17.46695   B1   70   0.00000     1541   152   GLN   C   -34.89656 -33.04752   17.46695   B1   70   0.00000     1542   152   GLN   C   -34.69656 -33.04752   17.46695   B1   70   0.00000     1543   152   GLN   C   -34.49656 -33.04752   17.46695   B1   70   0.00000     1544   152   GLN   C   -33.46155 -31.26900   18.60094   B1   70   0.00000     1545   152   GLN   C   -32.33676 -29.77012   118.6006   B1   70   0.00000     1546   152   GLN   MEZ   -34.46566 -29.2019   118.6006   B1   70   0.00000     1546   152   GLN   MEZ   -34.46566 -29.64602   118.57711   B1   70   0.00000     1547   152   GLN   MEZ   -34.28186 -28.63558   118.46911   B1   70   0.00000     1549   152   GLN   0   -37.09756 -32.85641   116.43607   B1   70   0.00000     1549   152   GLN   0   -37.09756 -32.85641   116.43607   B1   70   0.00000     1550   153   ANG   N   -35.34435 -33.30759   115.08552   B1   71   0.00000     1551   153   ANG   N   -35.34435 -33.30759   115.08552   B1   71   0.00000     1552   153   ANG   C   -34.8280 -32.07751   112.55554   B1   71   0.00000     1553   153   ANG   C   -33.84280 -32.07751   112.55554   B1   71   0.00000     1555   153   ANG   C   -33.84280 -32.07751   112.55554   B1   71   0.00000     1556   153   ANG   K   -33.7858   30.09360   10.5566   B1   71   0.00000     1556   153   ANG   K   -33.7858   30.09360   10.5566   B1   71   0.00000     1556   153   ANG   K   -33.7858   30.09360   10.5566   B1   71   0.00000     1557   153   ANG   K   -33.7858   30.09360   10.5566   B1   71   0.00000     1558   153   ANG   K   -32.57675   32.17691   108.83735   B1   71   0.00000     1556   153   ANG   K   -32.57675   32.17691   108.83735   B1   71   0.00000     1556   153   ANG   K   -32.57655   33.03805   114.36655   B1   71   0.00000	1534	151 GLU	OEl	-30.71320	0 -30.3312	9 117.58148 B1	69	0.00000
1537 153 CBU 0 -35.75790 -35.57313 17.58647 B1 69 0.00000 1539 152 GBN H -33.00321 -34.10256 1)7.18602 B1 70 0.00000 1541 152 GBN CB -34.186656 -33.04752 1)7.406958 1 70 0.00000 1541 152 GBN CB -34.186656 -33.04752 1)7.406958 1 70 0.00000 1541 152 GBN CB -34.15686 -33.04752 1)7.406958 1 70 0.00000 1541 152 GBN CB -34.15686 -33.04752 1)7.406958 1 70 0.00000 1542 152 GBN CB -33.213368 -29.27019 1)8.50038 B1 70 0.00000 1543 152 GBN CD -33.23376 -29.77424 118.49387 B1 70 0.00000 1544 152 GBN CB -33.213366 -29.27019 1)8.36008 B1 70 0.00000 1545 152 GBN ED -33.213366 -29.27019 1)8.36008 B1 70 0.00000 1546 152 GBN HEZZ -34.21656 -29.04682 1)8.54711 B1 70 0.00000 1546 152 GBN HEZZ -34.21686 -29.46521 1)8.36008 B1 70 0.00000 1547 152 GBN HEZZ -34.21686 -29.46521 1)8.36008 B1 70 0.00000 1547 152 GBN HEZZ -34.2168 -28.6555 B1 18.46563 B1 70 0.00000 1549 152 GBN REZZ -34.2168 -28.6555 B1 18.46507 B1 70 0.00000 1549 152 GBN REZZ -34.2168 -28.6555 B1 18.46563 B1 70 0.00000 1550 153 ARG N -35.34435 -33.30759 15.03552 B1 71 0.00000 1551 153 ARG R -34.35893 -33.42129 1)8.95976 B1 71 0.00000 1551 153 ARG CD -35.46322 -33.43707 112.65564 B1 71 0.00000 1555 153 ARG CD -35.46322 -33.43707 112.65564 B1 71 0.00000 1555 153 ARG CD -35.46322 -33.43707 112.65564 B1 71 0.00000 1555 153 ARG CD -35.46322 -33.14707 112.65564 B1 71 0.00000 1556 153 ARG CD -35.46322 -33.22570 111.17839 B1 71 0.00000 1556 153 ARG R -33.51371 -30.95305 110.55166 B1 71 0.00000 1556 153 ARG R -33.51371 -30.95305 110.55166 B1 71 0.00000 1556 153 ARG R HZ -33.78658 -30.09360 110.9860 B1 71 0.00000 1556 153 ARG R HZ -33.78658 -32.22570 111.17839 B1 71 0.00000 1566 153 ARG R HZ -33.78658 -30.09360 110.9860 B1 71 0.00000 1566 153 ARG R HZ -33.78658 -30.09360 110.9860 B1 71 0.00000 1566 153 ARG R HZ -33.78656 -30.09360 110.9860 B1 71 0.00000 1566 153 ARG R HZ -33.58669 -30.8260 HZ -30.8262 B1 71 0.00000 1566 153 ARG R HZ -33.5866 -30.8660 B1 8.5665 B1 71 0.00000 1566 153 ARG R HZ -33.5866 B1 72 0.00000 1566 153 ARG R HZ -33.5866 B1 72 0.00000 1566 153 ARG R HZ -33.5866				-30.51522	2 -38.5646	2 119.72459 B1		
1538   152 GLN   -33,08501 -34,19700   117,35586 B)   70				-34.55067	7 -35.4116	8 117.43857 Bl		
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1540   152 GLN   Ch   -34, 15680 -31, 71666   17, 20695   170   0.00000	1538		N	-33.98603	-34.1978	0 117.35586 B1		
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1557 153 ARG	1555	153 ARG	CD				71	0.00000
1558 153 ARG CZ	2556	253 ARG	NE	-33.53171	-30.95306	110.55166 B1	71	0.00000
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1591 155 ARG HE -41.63763 -33.16145 121.09517 81 73 0.00000 1592 155 ARG C2 -40.47069 -31.92135 122.22743 81 73 0.00000 1593 155 ARG NH1 -41.6382 -31.43599 122.94081 81 73 0.00000 1594 155 ARG HH11 -41.33886 -30.75247 123.65592 81 73 0.00000 1595 155 ARG HH12 -42.41818 -31.75018 122.77039 81 73 0.00000		155 ARG						
1592 155 ARG C2 -40.47089 -31.92135 122.22743 B1 73 0.00000 1593 155 ARG NH1 -41.46332 -31.43599 122.94081 B1 73 0.00000 1594 155 ARG NH1 -41.33886 -30.75247 123.65592 B1 73 0.00000 1595 155 ARG NH12 -42.41818 -31.75018 122.77639 B1 73 0.00000		155 ARG						
1593 155 ARG NH1 -41.65362 -31.43599 122.94681 81 73 0.00000 1594 155 ARG HH11 -41.33886 -30.75247 123.65592 81 73 0.00000 1595 155 ARG HH12 -42.41818 -31.75018 122.77639 81 73 0.00000		155 FDC						
1594 155 ARG HH11 -41.33886 -30.75247 123.65592 E1 73 0.00000 1595 155 ARG HH12 -42.41818 -31.75018 122.77039 E1 73 0.00000		755 EDG						
1595 155 ARG HH12 -42.41818 -31.75018 122.77039 51 73 0.00000								
		155 ARG						

FIG. 26



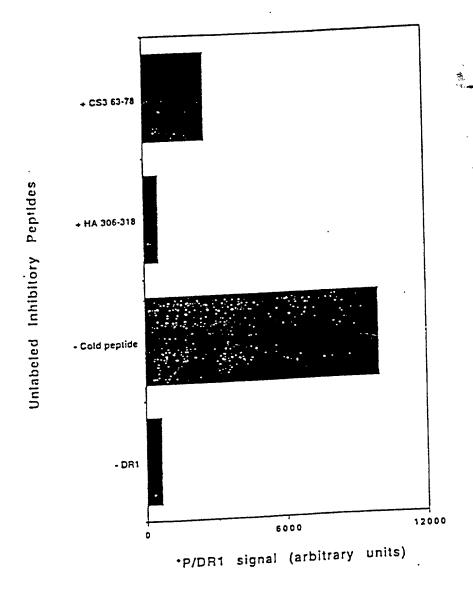
Jdr1\_MIN2.CRD Thu Feb 25 14:55:48 1993 26

_								
150		HH2		-30.51248	123,15141	B1	73	0.00000
1500		HH2: C	2 -38,47020 -40,65389	-31.56739 -36.07891	121.91409 118.56312	<b>51</b>	73	0.00000
1000		Õ	-41,80290	-36.51173	116,56408	<b>8</b> 1 81	73 73	0.00000
1601		Ň	-40.28792	-34.01372	115.84196	81	74	0.00000
1602		Ä	-39.31961	-33.75543	115.77185	61	74	0.00000
1003		CA	-41.30773	-33,34225	115.03220	B1	74	0.00000
1604	158 ALA	CB	-40,72899	-32.10061	114,35246	81	74	0.00000
1605	156 ALA	C	-41.91382	-34.25964	113.98113	<b>B</b> 1	74	0.00000
1606		0	-43.11961	-34.40603	113.83911	81	74	0.00000
1607		N	-40.99693	-34.92630	113.29026	81	78	0.00000
1806		H	-40.04150	-34,68633	113.44609	81	78	0.00000
1600		CA	-41.27013	-36.00533	112.34552	61	76	0.00000
1610 1611		CB CG1	-39.86851 -39.79482	-36.59697 -38.01333	112,04095	B1	75	0.00000
1612		CG2	-39.10167	-35.63993	111,48596 111,12688	B1 B1	78 75	0.00000
1613		Č	-42.31375	-37.01997	112.83333	B1	75 75	0.00000
1614		ŏ	-43.41565	-37.10246	112,30297	B1	78	0.00000
1618		Ň	-41.95945	-37.78157	113.57061	81	76	0.00000
1610	158 ASP	Н	-41.06306	-37.68674	114,30470	B1	76	0.00000
1617		CA	-49.85616	-35.64272	114,32359	<b>B</b> 1	76	0.00000
1518		CB	-42.00373	-39.82201	115.22733	B1	76	0.00000
1619		CG	-41.27306	-40.79302	114,39962	81	76	0.00000
1620 1621	158 ASP 158 ASP	OD1 OD2	-40.34839	-40.37834	113.70459	B1	76	0.00000
1022		C	-41,56822 -44,10643	-41,95359 -38,36708	114.41607	81	78	0.00000
1623		ŏ	-46,17033	-38.96720	115.04368 114.93521	81 81	76	0.00000
1624		N	-43.96505	-37.26912	115.79661	81	76 77	0,00000
1625	150 THR	Н	-43.09027	-36.78113	115.86564	<b>8</b> 1	77	0.00000
1626	159 THR	CA	-45.15804	-36.88791	116.55067	B1	77	0.00000
1627	150 THR	CB	-44.86388	-36.97162	118.07412	B1	77	p.00000
1628	159 THR	001	-46.06916	-37.10322	118.79712	51	77	0.00000
1629	160 THR	HG1	-48.91547	-37.30001	119.72205	B1	77	0.00000
1630 1631	159 THR 159 THR	C@2 C	-44.03422	<b>-35.82624</b>	118,66004	81	77	0.00000
1632	159 THR	ŏ	-45,84469 -47,06168	<b>-38.59</b> 150	110.12007	B1	77	0.00000
1633	160 TYR	N	-45.05289	-35.51846 -34.54372	118.90788	81	77	0.00000
1634	160 TYR	Ĥ	44.06861	-34.64495	115,67045 115,76833	81 81	78	0.00000
1635	160 TYR	CA	-45,73493	-33.26691	115.64251	81	78 78	0.00000 0.00000
1636	160 TYR	CB	-44.74473	-32,10748	118.78676	B1	78	0.00000
1637	160 TYR	CG	-48.25402	-31.12365	116.81319	81	78	0.00000
1638	160 TYR	CD1	<b>-44.85214</b>	-31.25680	118,16144	B1	78	0.00000
1639 1640	160 TYR 160 TYR	CE1	-45,32019	- <b>30.34310</b>	110.12626	B1	78	0.00000
1641	160 TYR	CE3 CD3	-46.12744 -46.60347	-30.08443	116.42011	B1	78	0.00000
1642	160 TYR	CZ	-46.20180	-29.17117 -29.30408	117.38468	81	78	0.00000
1643	160 TYR	OH	-46.66272	·28.41253	116,73381 119,68223	81 81	78	0.00000
1644	160 TYR	HH	-47.28242	-27.80044	119.27249	B1	78 78	0.00000 0.00000
1645	160 TYR	C	-46.46000	-33,18254	114,31073	B1	78	0.00000
1646	160 TYR	0	-47.63057	-32.82968	114.21477	Bi	70	0.00000
1647	161 CYS	N	-46.72598	-33.58992	113.36774	<b>B1</b>	79	0.00000
1649	161 CYS 161 CYS	H Ca	-44.77052 -46.32703	-33.85209	113.40718	81	79	0.00000
1050	161 CY8	CB	48.27134	-33.68877 -34.17403	111.93544	81	79	0.00000
1681	161 CY8	8G	-48.67068	-34.17403 - <b>33.837</b> 16	110.93068	81	79	0.00000
1662	161 CY8	C	-47.53731	-34.60219	109.19024 111.93094	81 B1	79 70	0.00000
1653	161 CYS	0	48.58723	-34,29704	111.38273	B1	75 75	0.00000
1664	162 ARG	N	-47.37462	-35.72008	112.66592	81	80	0.00000
1668	162 ARG	H	-46.47838	-35.94232	113.03662	81	80	0.00000
1666 1667	162 ARG 162 ARG	CA	-48.50678	-30.61784	112.89068	81	80	0.00000
1668	162 ARG	CE	<b>-48.077</b> 10	-37.71819	113.85476	81	ģΟ	0.00000
1669	102 ARG	CD	-49.16340 -48.67644	-38,77197 -40,04247	114.12227	B1	80	0.00000
1660	162 ARQ	NE	-49.62321	-40.04247 -41,12379	114.81623	81	80	0.00000
				7 * 7 1 <b>= 4 1 #</b>	114.54199	81	86	0.00000

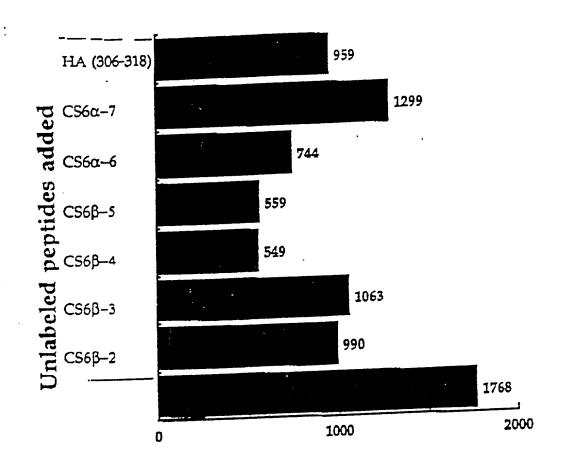
./071	_אבאי2 . כא	5	Thu Feb	25 14:50:	48 1993	27	
1661	162 AR	C HE	-50. 9	4 -40 8945	5 114.11092 B1	28	0.00000
1662					7 114.80601 Bi	80	0.00000
1663		_			4 114.46730 B1	80	0.00000
1664			1 -50.1197			80	0.00000
1665			2 -51.0618			80	0.00000
1666	162 ARG				3 115.38323 B1	80	0.00000
1667	162 ARC		1 -48.0013			80	0.00000
1668	162 ARC			9 -42.0678		80	0.00000
1669	162 ARG				6 113.42487 B1	80	0.00000
1670	162 ARG	_		3 -35.9373		80	0.00000
1671	163 HIS			3 -35.3186		81	0.00000
1672	163 HIS			2 -35.2803		81	0.00000
1673	163 HIS			1 -34.7335		81	0.00000
1674	163 HIS				5 116.66134 B1	81	0.00000
1675	163 HIS			6 -35.5064		81	0.00000
1676	163 HIS				2 118.12240 B1	81	0.0000
1677	163 HIS	HD1		0 -35.6743		81	0.00000
1678	163 HIS	CD2		4 -36.28831		81	0.00000
1679	163 HIS	NE2			9 118.73130 Bl	81	0.00000
1680	163-HI6				-118.84798 B1	81	0.00000
1681	163 HIS	C			114.44466 B1	81	0.00000
1682	163 HIS	ō			114.18659 B1	81	0.00000
1663	164 ASN	N			5 114.01202 B1	82	0.00000
1684	164 ASN	H			2 114.21247 B1	82	0.00000
1685	164 ASN	CA			113.20331 B1	82	0.00000
1686	164 ASN	CB	-49.96583	3 -30.54363	112.89196 B1	82	0.00000
2687	264 ASN	CG.	-49.91907	-29.53869	114.02377 B1	82	0.00000
1688	164 ASN	OD1	49.13948	-29.62233	3 114.96163 B1	82	0.00000
1689	164 ASN	NDS	-50.80473	-28.55321	. 113.91309 B1	82	0.00000
1690	164 ASN	HD21			113.14586 B1	82	0.00000
1591	164 ASN	HD22			114.61251 B1	82	0.00000
1692	164 ASN	С	-51.70674	-32.02333	111.91584 B1	82	0.00000
1693	164 ASN	0			111.51085 B1	82	0.00000
1694	165 TYR	N			111.29191 B1	83	0.00000
1695	165 TYR	H			111.62194 B1	83	0.00000
1696 1697	165 TYR	CA		-33.54191		83	0.00000
1698	165 TYR 165 TYR	CB CG		-34.47239		83	0.00000
1599	165 TYR	CD1		-34.50284		83	0.00000
1700	165 TYR	CEI		-33.44669 -33.47413		83 83	0.00000 0.00000
1701	165 TYR	CD2			106.96903 B1	83	0.00000
1702	165 TYR	CE2			105.62740 B1	83	0.00000
1703	165 TYR	CZ		-34.55457		83	0.00000
1704	165 TYR			-34.53152		83	0.00000
1705	165 TYR	нн		-34.97162		83	0.00000
1706	165 TYR	С	-53.16114	-34.17050	110.39688 B1	83	0.00000
1707	165 TYR	0		-33.75040		83	0.00000
1708	166 GTA	N	-53.16827	-35.13255	111.32677 B1	84	0.00000
1709	166 CTA	H	-52,30920	-35.44284	111.74443 B1	84	0.00000
1710	166 CTA	CA			111.69489 E1	84	0.00000
1711	166 GTA	С	-55.55421	-34.78683	112.08191 B1	84	0.00000
1712	166 CTA	0			111.64884 B1	84	0.00000
1713	167 VAL	N			112.90998 B1	85	0.00000
1714	167 VAL	H			113.25020 B1	85	0.00000
1715	167 VAL	CA			113.26808 B1	85	0.00000
1716	167 VAL	CB			114.36486 B1	85	0.00000
	167 VAL	CG1			114.75691 81	85	0.00000
	167 VAL 167 VAL	CGZ			115.60849 B1	85	0.00000
	167 VAL	0		-31.96437	112.06515 B1	85	0.00000
1721	168 GLY	33			111.87375 B1 111.20320 B1	85 86	0.00000
	168 GLY	H	-54.68827		111.20320 B1	86	0.00000
:723	158 GLY	CA.			109.94972 B1	86	0.00000
	168 GLY	c			109.11607 81	86	0.00000

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1725	168 GLY	0	-58. 45	-31.28044	108 61617	B1 86	0.00000
1726	169 GLU	N	-56.7:134	-33.07169	109.00665	B1 87	0.00000
1727	169 GLU	н		-33.43085			0.00000
1728	169 GLU	CA	-57.59179	-34.00467	108.30469		0.00000
1729	169 GLU	СB		-35.39155			0.00000
1730	169 GLU	CG	-55.67851	-35.40281	107.43481	B1 87	0.00000
1731	169 GLU	CD		-36.69049			0.00000
1732	169 GLU	OE1	-53.74095	-36.61342	108.02205	B1 87	0.00000
1733	169 GLU	OE2		-37.76250			0.00000
1734	169 GLU	C		-34.05273			0.00000
1735	169 GLU	0	-59.98966	-34.06690 -33.99305	110 19884		0.00000
1736 1737	170 SER 170 SER	Н	-59.00330	-34.05998	110.74831		0.00000
1738	170 SER	CA			110.83391		0.00000
1739	170 SER	CB			112.35798		0.00000
1740	170 SER	OG	-61.42043	-34.13237	113.03659		0.00000
1741	170 SER	НG		-34.00943			0.0000
1742	170 SER	С		-32.61665			0.00000
1743	170 SER	0		-32.69150			0.00000
1744	171PHE			-31.45621			0.00000
1745	171 PHE	Н		-31.41832			0.00000
1746	171 PHE	CA		-30.24631	109.95663		0.00000
1747	171 PHE	CB		-28.99941	110.10880		0.00000
1748 1749	171 PHE 171 PHE	CG		-28.68147 -28.39703	111.85413		0.00000
1750	171 PHE	CD1 CD2		-28.63398	112.55491		0.00000
1751	171 PHE	CEI		-28.06074	113.17656		0.00000
1752	171 PHE	CE2		-28.29967	113.87858		0.00000
1753	171 PHE	CZ		-28.01319	114.18527	_	0.00000
1754	171 PHE	Ċ		-30.29139	108.49502		0.00000
1755	171 PHE	Ο.	-62.68697	-29.84047	108.07691	B1 89	0.00000
1756	172 THR,	N,	-60.72520	-30.85206	107.69903		0.00000
1757	172 THR	H		-31.29854	108.09636		0.00000
1758	172 THR	CA		-30.66246	106.25599		0.00000
1759	172 THR	CB		-30,70747	105.70165		0.00000
1760 1761	172 THR 172 THR	0G1		-30.21143 -30.48800	104.36207		0.00000
1762	172 THR	HG1 CG2		-32.13906			0.00000
1763	172 THR	c		-31.64677			0.00000
1764	172 THR	ŏ		-31.56505	104.25169		0.00000
1765	173 VAL	N		-32.60764	106.19315		0.00000
1766	173 VAL	H		-32.56397	107.19363	B1 91	0.00000
2767	173 VAL	CA	-62.87984	-33.81113	105.53718	B1 91	0.00000
1768	173 VAL	CB		-34.51911	106.47899		0.00000
1769	173 VAL	CG1		-35.77324	105.85034		0.00000
1770 1771	173 VAL	CG2		-34.90248	107.79466		0.00000
1772	173 VAL 173 VAL	C	-63.51710		104.16716		0.00000
1773	174 GLN	0 N		-34.24452 -32.59570	103.18126		0.00000
1774	174 GLN	Я		-32.11269			0.00000
1775	174 GLN	CA		-32.19104			0.00000
1776	174 GLN	CB	-65.76132	-30.80951	103.22574		0.00000
1777	174 GLN	ÇG		-30.26016			0.00000
1778	174 GLN	CD	-66.09397	-29.58024	101.04012	B1 92	0.00000
1779	174 GLN	OE1		-28.54065			0.00000
1780	174 GLN	NE2	-66.26402		99.67453		0.00000
1781	174 GLN		-66.63226		99.82928		0.00000
1762	174 GLN		-65.97833		99.02730		0.00000
1783 1784	174 GLN 174 GLN	C		-32.18074 -32.51356	101.63553		0.00000
1785	174 GER	0		-32.31336	101.73327		0.00000
1786	175 ARG	H		-31.53564	102.62225		0.00000
1787	175 ARG	C.A.	-62.31707		100.50018		0.00000
1788	175 ARG	CB		-30.36631	100.16958	B1 93	0.00000

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1789		CG	-61.2439	5 -30.2691		93	0.00000
1790		CD		7 -28.0420		93	0.00000
1791		NE		7 -28.8721		93	0.00000
1792		HE		6 -29.7691		93	0.00000
1793		CZ		5 -27.7492		93	0.00000
1794	175 ARG			3 -27.83579		93	0.0000
1795	175 ARG			4 -27.0272		93	0.00000
1796	175 ARG			0 -28.7345		93	0.00000
1797	175 ARG	NH2		7 -26.55682		93	0.00000
1798	175 ARG			B -25.70796		93	0.00000
1799	175 ARG 175 ARG			1 -26.50975		93	0.00000
1800		C		6 -32.79150		93	0.0000
1801	175 ARG	0		7 -33.52736		93	0.00000
1802	176 ARG	N		3 -32.85103		94	0.00000
1803	176 ARG	H		-32.31340		94	0.00000
1804	176 ARG	CA		-33.80802		94	0.00000
1805	176 ARG	CB		-33.62483		94	0.00000
1806	176 ARG	CG			102.34974 B)	94	0.00000
1807 1808	176 ARG	8		-32.28237		94	0.00000
1509	176 ARG 176 ARG	NE		-30.9401B		94	0.00000
1810	176 ARG	HE		~30.25818		94	0.00000
1911	176 ARG	CZ NH1		-30.63659		94	0.00000
1812	176 ARG	HH11		-29.38340 -29.10955	105.64628 B1	94 94	0.00000
1813	176 ARG			-28.69008		94	0.00000
1814	176 ARG	NH2			105.89297 B1	94	0.00000
1315	176 ARG			-31.37726		94	0.00000
1816	176 ARG	нн22			105.54660 B1	94	0.00000
1817	176 ARG	С		-35,27348		94	0.00000
1818	176 ARG	ō			101.06767 B1	94	0.00000
1819	177 VAL	N			101.85272 B1	95	0.00000
1820	177 VAL	H		-34.82991		95	0.00000
1521	177 VAL	CA			101.70299 B1	95	0.00000
1822	177 VAL	С3 .		-37.47193		95	0.00000
1823	177 VAL	CG1		-39.00335		95	0.00000
1824	177 VAL	CG2		-37.00753		95	0.00000
1525	177 VAL	С	-62.41412	-37.02458	100.63553 B1	95	0.00000
1826	177 VAI	0	-63.44404	-37.67295	100.79118 B1	95	0.00000
1627	178 HIS	N	-62.14889	-36.33028	99.52296 B1	96	0.00000
1828	178 HIS	н	-61.32158	-35.77698	99.39184 B1	96	0.00000
1829	178 HIS	CA	-63.09845	-36.32813	98.41659 B1	96	0.00000
1830	178 HIS	CB	-64.01495	-35.10064	98.57314 B1	96	0.00000
1631	178 HIS		-65.27852	-35.21481	97.74669 B1	96	0.00000
1632				-35.62002	96.46944 Bl	96	0.00000
1833	178 HIS			-35.91855	95.96816 Bl	96	0.00000
1834	178 HIS			-34.92566	98.14872 B1	96	0.00000
1635	178 HIS			-35.16505	97.08780 B1	96	0.00000
1836 1837	178 HIS			-35.59364	96.05191 Bl	96	0.00000
1838	178 HIS 178 HIS			-36.29235	97.09131 B1	96	0.00000
1639	178 HIS	OCT1	-61.22615	-35.78756	97.07091 Bl	96	0.00000
		0012	- 02.8/363	-36.77415	96.08799 Bl	96	0.00000



## Inhibition of 125 I HA (306-318)/DRI by unlabeled CSG of and B peptides



\*HA/DR1 compact dimer signal (densitometric units)